ALGEBRAIC SOLUTIONS TO THE THOMAS-FERMI EQUATION FOR ATOMS

Thesis submitted by
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Declaration

I hereby declare that the following thesis is based on research carried out by me, that the Thesis is my own composition, and that it has not been presented previously for a higher degree.

CERTIFICATE

I certify that Ir. P.J. Rijnierse has spent nine terms as a research student in the Department of Theoretical Physics of the United College of St. Salvator and St. Leonard in the University of St. Andrews, that he has fulfilled the conditions of Ordinance No. 16 of the University Court of St. Andrews and that he is qualified to submit the accompanying Thesis in application for the Degree of Doctor of Philosophy.

Research Supervisor

Career

From 1958 to 1964 I studied at the Technical University of Delft, Netherlands, and in 1964 I was awarded the degree of Physical Engineer (M.Sc. in Physical Engineering) cum laude. In the last year of this course I was financially supported by an assistant ship to Professor R. Kronig in the Department of Technical Physics.

In October, 1964 I was offered a S.R.C. Research Assistantship tenable in the Department of Theoretical Physics in St Salvator's College of the University of St Andrews. Since that time I have been engaged in research on the subject of this thesis.
In October 1965 I registered as a research student in the Faculty of Science, St Salvator's College, and as a candidate for the degree of Doctor of Philosophy. From the same time, I have held a University Research Assistantship in the Department of Theoretical Physics, which expired on January 1st, 1968. Since then I have been engaged in research in Philips Research Laboratories, Eindhoven, Netherlands, on the subject of magnetic materials and their suitability as components in computer memory devices.

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CONTENTS

INTRODUCTION

The main purpose of this work is to study the mathematical aspects of the Thomas-Fermi (TF) statistical model of electrons in atoms. The emphasis is on expansions converging sufficiently fast to yield accurate numerical results.

After a brief review of the theoretical basis of the TF model (ch. 1) and a survey of the methods employed by previous workers to solve the TF equation (ch. 2), a summary of the methods applied and the results obtained in this work is presented in chapter 3. Chapters 4-7 are devoted to a detailed analysis of the TF equation for the isolated and for the moderately compressed atom, while in chapter 8 the extremely compressed atom is treated.

The techniques applied, especially for the solution of two-point boundary value problems and for the analysis of functions with the help of their series expansions, are not limited to this particular problem: in ch. 9 we consider a number of problems in physics where we feel they could be succesfully applied. Finally, some numerical results and some purely mathematical considerations are collected as appendices in ch. 10.

The theory describes the electrons in an atom as a completely degenerate gas with only electron-electron and electron-nucleus Coulomb interaction. If the potential V varies slowly and the electron density ρ is high enough, then a spherically symmetric atom is described by the solution $\varphi(x)$ of the dimensionless TF equation

$$\frac{d^2\varphi}{dx^2} = x^{-\frac{1}{2}}\,\varphi^{\frac{3}{2}} \quad . \tag{I}$$

In this equation φ is connected with V and ρ by the relations

$$V = \frac{Ze\varphi}{\mu x} + V_0 \quad , \quad \rho = \frac{Z}{4\pi\mu^3}\left(\frac{\varphi}{x}\right)^{\frac{3}{2}} \quad ;$$

Z is the atomic number, $-eV_0$ the highest electron energy in the atom and $r = \mu x$ the distance from the nucleus with

$$\mu = \left(\frac{3}{32\pi^2}\right)^{\frac{1}{3}} \frac{\hbar^2}{2me^2 Z^{\frac{1}{3}}} \quad .$$

For an isolated atom x ranges from 0 to ∞ and the boundary conditions are

$$\text{(a)} \quad \varphi(0) = 1 \qquad ; \text{(b)} \quad \varphi(\infty) = \varphi'(\infty) = 0 . \qquad \text{(II)}$$

For a compressed atom of atomic volume $v = \frac{4}{3}\pi \lambda_0^3 = \frac{4}{3}\pi \mu^3 x_0^3$ one has $0 \leq x \leq x_0$ and the boundary conditions are

$$\text{(a)} \quad \varphi(0) = 1 \qquad ; \text{(b)} \quad \varphi(x_0) = x_0 \varphi'(x_0) . \qquad \text{(III)}$$

The fact that both (II) and (III) are two-point boundary conditions is the root of most of the difficulties encountered, together with the non-linearity of the basic equation (I). Our method of solution consists in expanding, at either end of the range of x, the TF function φ as a function satisfying the appropriate boundary condition. The resultant one-parameter solutions, each valid in a different region of x-values, are then matched at some intermediate point, for which we have chosen $x = 1$ throughout this work.

Since (IIa) and (IIIa) are identical, φ can be expanded around $x = 0$ in the same way for both isolated and compressed atoms. Choosing $\mathcal{B} \equiv \varphi'(0)$ as a parameter, one obtains a one-parameter family of solutions $\varphi(x, \mathcal{B})$, the so-called Baker [1] series solution. For the isolated-atom value $\mathcal{B} = -1.588071022 6$ the series ceases to converge beyond $x = 0.4$; however, we show that for any given, fixed, value of x we can write φ and φ' as a power series in $\mathcal{B}$. In particular, we choose for this fixed point $x = 1$: the expansions of $\varphi(x=1, \mathcal{B})$ and $\varphi'(x=1, \mathcal{B})$ are calculated once and for all and for any value of $\mathcal{B}$ one easily finds $\varphi(1)$ and $\varphi'(1)$.

For the isolated atom, the condition (IIb) leads to a one-parameter solution commonly known as the Coulson-March (CM)

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1) E.B. Baker, Phys.Rev. 36 (1930) 630-47.

asymptotic solution [2]. In its original form, the CM series for the isolated atom - with the value $F = 13.270973848$ for the parameter - converges down to $x \approx 4.75$, but the convergence is too slow for numerical summation unless $x \gtrsim 10$. However, we have been able to recast this series into a form where it yields 5-place accuracy for x as small as 0.6.

The isolated-atom values of $\mathcal{B}$ and F can now be determined by requiring that φ and φ' as determined from the Baker or CM solutions are continuous across $x = 1$.

For the compressed atom, a generalization of the CM solution due to Gilvarry and March [3] yields a two-parameter family of solutions which can again be cast into a form which converges sufficiently fast for numerical application at $x = 1$. The condition (IIIb) eliminates one of the parameters; the matching conditions at $x = 1$ determine $\mathcal{B}$ and the other parameter. Thus expansions for the CMG-parameters, $\mathcal{B}$ and $\varphi(x_0)$ in terms of the boundary radius x_0 are obtained.

Since this last method rests on the fact that x_0 is large, it fails for highly compressed atoms ($x_0 \lesssim 1$). We then resort to a completely different technique [4], converting (I) into an integral equation under insertion of the boundary condition (IIIb). By a method of successive approximations a solution is obtained in which the parameter is determined by the condition (IIIa).

Though only the zero-temperature case is treated, our algebraic expressions will presumably be applicable also in the non-zero-temperature perturbation treatment, where Gilvarry [5] shows how the perturbed TF function may be obtained from the unperturbed one by simple quadratures. The numerical results of similar work by Feynman et.al.[6] must be treated as unreliable since their values for the unperturbed TF function already show severe errors.

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2) C.A. Coulson and N.H. March, Proc.Phys.Soc.A 63 (1950) 367-74; N.H. March, Proc.Camb.Phil.Soc. 48 (1952) 665-82.

3) J.J. Gilvarry and N.H. March, Phys.Rev. 112 (1958) 140-9, referred to as GM; this solution is referred to as the Coulson-March-Gilvarry (CMG) solution.

4) P.J. Rijnierse, Proc.Roy.Soc. A292 (1966) 288-97.

5) J.J. Gilvarry, Phys.Rev. 96 (1954) 934-43 and 944-8.

6) R.P. Feynman, N. Metropolis & E. Teller, Phys.Rev. 75 (1949) 1561-73.

We will not attempt to give an exhaustive account of all recent applications of TF theory; a few examples may serve as an indication of its continued interest, in spite of its obvious weaknesses. They include the calculation of the overlap energy between rare gas atoms [7] and the high pressure behaviour of these gases [8]; the photo-electric cross-section of atoms [9]; the binding energy [10] and the energy levels [11] of electrons in atoms and in positive ions.

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7) O.B. Firsov, Soviet Phys.JETP 5 (1957) 1192-6;
R.D. Present, J.Chem.Phys. 47 (1967) 1793-9. (no.5, 1 sept).
8) M. Ross & B. Alder, J.Chem.Phys. 47 (1967) no.10, 15 nov.,4129-33.
9) G. Rakavy & A. Ron, Phys.Rev. 159 (1967) 50-6.
10) D. Shalitin, Phys.Rev. 140 (1965) A1857-63;
Phys.Rev. 155 (1967) 20-3.
11) A. Jain & S. Kumar, Canad.J.Phys. 45 (1967) 1745-54 (no.5, May).

CHAPTER 1 . THEORETICAL BASIS OF THE THOMAS-FERMI MODEL FOR ATOMS

We will review the basic features of the statistical treatment of the electron gas originally due to Thomas [1] and Fermi [2], and of the extension to it due to Dirac [3]. Much more extensive references and discussions may be found in the book by Gombás [4] and in review articles by Gombás [5] and March [6].

1.1 . The Thomas-Fermi model in general

The essential assumptions of the model are:

(i) the electrons form a completely degenerate electron gas;

(ii) the electron density is so high that the gas can be treated as a continuous charge distribution, satisfying Poisson's equation;

(iii) only electrostatic interactions between the electrons are taken into account;

(iv) the interaction can be entirely described by an average potential which varies so slowly that the electrons can be treated as locally free;

(v) the electron distribution and the potential determine each other in a self-consistent way.

Two obvious weaknesses follow immediately from these assumptions: because of (ii) the model breaks down in regions of low density such as in light atoms or in the outer regions of heavy atoms, while (iv) causes the theory to fail near nuclei, where high potential gradients occur.

The basic TF equation will be derived from a variational principle [7]. The electron coordinate space is divided into small "cells" of size $d\underline{\lambda}$ at $\underline{\lambda}$. The size of these cells is chosen so as

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1) L.H. Thomas, Proc.Camb.Phil.Soc. 23 (1927) 542-8.

2) E. Fermi, Z.f.Phys. 48 (1928) 73-9.

3) P.A.M. Dirac, Proc.Camb.Phil.Soc. 26 (1930) 376-85.

4) P. Gombás, Die statistische Theorie des Atoms und ihre Anwendungen, Springer, Vienna, 1949.

5) P. Gombás, Statistische Behandlung des Atoms, in Handb.d.Phys. 36 (1956) 109-231.

6) N.H. March, Adv.in Phys. 6 (1957) 1-101.

7) J. Frenkel, Z.f.Phys. 50 (1928) 234-48.

to satisfy (ii) and (iv) simultaneously. In each cell, by (iv), the electron energy is given by the free electron value at the local density: by summing over all cells (= integrating over all space) we obtain the total energy. The TF density is now determined by minimizing the energy, keeping the nuclei fixed in space and the total charge constant.

For the kinetic energy E_{kin} one finds in this way

$$E_{kin} = c_k \int \rho^{\frac{5}{3}} \, d\underline{r} \quad , \tag{1.1. 1}$$

where the integration is over all accessible space, $\rho(\underline{r})$ is the density at $\underline{r}$, and

$$c_k = \left(\frac{3}{8\pi}\right)^{\frac{2}{3}} \frac{3h^2}{10m} \quad . \tag{1.1. 2}$$

To find the potential energy E_{pot} the potential $V(\underline{r})$ is written as

$$V = V_n + V_e \quad . \tag{1.1. 3}$$

Here V_n is the potential due to the nuclei and V_e that due to the electron cloud:

$$V_e(\underline{r}) = -e \int \frac{\rho(\underline{r}')}{|\underline{r}' - \underline{r}|} \, d\underline{r}' \quad . \tag{1.1. 4}$$

Introducing a factor $\frac{1}{2}$ in front of V_e to avoid double counting of electron pairs leads to

$$E_{pot} = -e \int (V_n + \tfrac{1}{2} V_e) \rho \, d\underline{r} \quad . \tag{1.1. 5}$$

The requirement that the total charge be constant introduces an additional condition

$$e \int \rho \, d\underline{r} = Ne \quad , \tag{1.1. 6}$$

where N is the (constant) total number of electrons.

With V_0 a Lagrangian multiplier, the variational principle takes the form

$$\delta (E + Ne V_0) \equiv \delta (E_{kin} + E_{pot} + Ne V_0) = 0 \quad . \tag{1.1. 7}$$

Varying ρ one finds the relation between ρ and V

$$\rho = \sigma_0 (V - V_0)^{\frac{3}{2}} \qquad (1.1.8)$$

with

$$\sigma_0 = \frac{8\pi}{3} \left(\frac{2me}{h^2}\right)^{\frac{3}{2}} . \qquad (1.1.9)$$

Since ρ and V also obey Poisson's equation we finally arrive at the TF equation:

$$\nabla^2 (V - V_0) = 4\pi e \sigma_0 (V - V_0)^{\frac{3}{2}} . \qquad (1.1.10)$$

The meaning of the Lagrangian multiplier V_0 can most easily be seen from the original argument of Thomas [1] and Fermi [2]. Since the electron gas is completely degenerate, the local fermi-momentum and the local density are connected by

$$\rho(\underline{r}) = \frac{8\pi}{3h^3} p_F^3(\underline{r}) . \qquad (1.1.11)$$

On the other hand the local maximum kinetic energy is connected with the maximum electron energy E_0 by

$$\frac{p_F^2(\underline{r})}{2m} - e V(\underline{r}) = E_0 \qquad (1.1.12)$$

so that

$$\rho(\underline{r}) = \frac{8\pi}{3h^3} \left\{2m(eV + E_0)\right\}^{\frac{3}{2}} . \qquad (1.1.13)$$

With $E_0 = -eV_0$ this is identical with (1.1. 8) and thus $-eV_0$ is the highest electron energy in the system.

1.2 . Atoms with spherical symmetry: isolated and compressed atoms

A significant simplification occurs if one assumes that potential and density are spherically symmetric. The nucleus of charge $+Ze$ is taken as the origin. Obviously very near the origin the potential will be that of the bare nucleus, therefore we write

$$V - V_0 = \frac{Ze}{r} \varphi(\underline{r}) \quad , \quad \varphi(0) = 1 \quad . \qquad (1.2.1)$$

If also

$$r = \mu x \quad , \quad \mu = \left(\frac{3}{32\pi^2}\right)^{\frac{2}{3}} \frac{\hbar^2}{2me^2 Z^{\frac{1}{3}}} \qquad (1.2.\ 2)$$

equation (1.1.10) reduces to the <u>dimensionless TF equation</u>:

$$\frac{d^2\varphi}{dx^2} = x^{-\frac{1}{2}} \varphi^{\frac{3}{2}} \quad . \qquad (1.2.\ 3)$$

In terms of φ the potential and the density can be written as

$$(a) \quad V = \frac{Ze}{\mu} \frac{\varphi}{x} + V_0 \; ; \; (b) \quad \rho = \frac{Z}{4\pi\mu^3} \left(\frac{\varphi}{x}\right)^{\frac{3}{2}} . \qquad (1.2.\ 4)$$

The total energy follows from (1.1. 1) and (1.1. 5) as

$$E = \frac{Z^2 e^2}{\mu} \left\{ \frac{1}{2} \varphi'(0) + \frac{1}{10} \int_0^{x_0} x^{-\frac{1}{2}} \varphi^{\frac{5}{2}} dx \right\} . \qquad (1.2.\ 5)$$

Here x_0 is the outer radius of the atom, and $v = \frac{4}{3}\pi\mu^3 x_0^3$ is the atomic volume. The integration can be explicitly performed following a method essentially due to Milne [8] to yield

$$E = \frac{Z^2 e^2}{\mu} \left\{ \frac{3}{7} \varphi'(0) + \frac{2}{35} x_0^{\frac{1}{2}} \varphi^{\frac{5}{2}}(x_0) \right\} . \qquad (1.2.\ 6)$$

The condition (1.1. 6) is easily seen to lead to

$$\varphi(x_0) - x_0 \varphi'(x_0) = \frac{Z - N}{Z} \quad . \qquad (1.2.\ 7)$$

First let us consider an isolated neutral atom, for which $N = Z$ and thus the right-hand side of (1.2. 7) vanishes. To make our description complete we must also know the value of the atomic boundary radius x_0 . The simplest way to find this value is to require that at the boundary the pressure must be zero, since otherwise the atom would be unstable. The pressure is that of a free electron gas of density $\rho(r_0)$, where $r_0 = \mu x_0$, so that $p = \frac{2}{3} e_k \rho^{\frac{5}{3}}(r_0) = 0$. Hence from (1.2. 4) we conclude

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8) E.A. Milne, Proc.Camb.Phil.Soc. <u>23</u> (1927) 794-9.

$$\varphi(x_0) = 0 \quad , \tag{1.2. 8}$$

and from (1.2. 7):

$$\varphi'(x_0) = 0 \quad . \tag{1.2. 9}$$

From the differential equation (1.2. 3) it now follows immediately that all derivatives $\varphi^{(n)}(x_0) = 0$. This leaves only two possibilities: either $\varphi(x) \equiv 0$ which is trivial, or $x_0 = \infty$. Thus for the isolated atom one has the conditions

$$0 \leq x < \infty \quad , \quad \varphi(0) = 1 \quad , \quad \varphi(\infty) = \varphi'(\infty) = 0 \quad . \tag{1.2.10}$$

Furthermore we find that

$$E = \frac{3}{7} \frac{Z^2 e^2}{\rho} \varphi'(0) \quad . \tag{1.2.11}$$

and from (1.2. 4a) it follows that $V_0 = V(\infty) = 0$.

Next let us treat atoms "compressed" inside a solid. Here there is no rigorous central symmetry. However, to quite a good approximation we can make use of Wigner and Seitz's [9] "atomic sphere" concept. The atom surrounding a given nucleus is assumed to be bounded by a regular polyhedron; its planes bisect the lines connecting the nucleus with its nearest and next-nearest neighbours and therefore the electric field vanishes on the midpoints of these planes. Since the atom is electrically neutral one expects the field of nucleus + electrons to be very small outside its own polyhedron. Thus it is consistent to assume that the field inside the atom is determined solely by its own electron distribution and that it is spherically symmetric in first approximation. We replace the polyhedron by a sphere of the same volume

$$V = \frac{4}{3} \pi r_0^3 \quad , \quad r_0 = \rho \, x_0 \quad . \tag{1.2.12}$$

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9) E. Wigner and F. Seitz, Phys.Rev. 43 (1933) 804-10 and 46 (1934) 509-24.

Now of course the pressure does not vanish, but is determined by the assumed atomic volume. For the compressed atom we thus arrive at

$$0 \leq x \leq x_0 \quad , \quad \varphi(0) = 1 \quad , \quad \varphi(x_0) = x_0 \varphi'(x_0) . \qquad (1.2.13)$$

The energy is

$$E = \frac{Z^2 e^2}{\nu} \left\{ \frac{3}{7} \varphi'(0) + \frac{2}{35} x_0^{\frac{1}{2}} \varphi^{\frac{5}{2}}(x_0) \right\} , \qquad (1.2.14)$$

again by Milne's [8] method, while with (1.2. 4b) the pressure is given by

$$p v = \frac{2 Z^2 e^2}{15 \nu} x_0^{\frac{1}{2}} \varphi^{\frac{5}{2}}(x_0) . \qquad (1.2.15)$$

It turns out that the method adopted in chapter 8 to solve the TF equation with the boundary conditions (1.2.13) for the extreme case where $x_0 \lesssim 1$ is applicable to a more general model, incorporating the exchange interaction. In the next section we will therefore discuss the Thomas-Fermi-Dirac (TFD) model.

1.3 . Inclusion of exchange: the Thomas-Fermi-Dirac model

The exchange interaction was first introduced into the statistical theory by Dirac [3], who proceeded in a manner analogous to that of equations (1.1. 11-13). The derivation becomes much simpler, however, if one extends the variational principle of section 1.1 , following Jensen [10]. A third term is added to the energy, the exchange energy E_{ex} of the free electron gas:

$$E_{ex} = - c_e \int \rho^{\frac{4}{3}} \, d\underline{r} \qquad (1.3. 1)$$

with

$$c_e = \frac{3}{4} e^2 \left(\frac{3}{\pi}\right)^{\frac{1}{3}} . \qquad (1.3. 2)$$

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10) H. Jensen, Z.f.Phys. 89 (1934) 713-9.

The variational principle now becomes

$$\delta(E + N_e V_0) \equiv \delta(E_{kin} + E_{pot} + E_{ex} + N_e V_0) = 0 \,, \qquad (1.3.\ 3)$$

where E_{kin} and E_{pot} are still given by (1.1. 1) and (1.1. 5), and by varying ρ one finds this time that

$$\rho = \sigma_0 \left\{ (V - V_0 + a^2)^{\frac{1}{2}} + a \right\}^3 , \quad a = \left(\frac{2me^3}{\hbar^2} \right)^{\frac{1}{2}} . \qquad (1.3.\ 4)$$

The positive sign for the square root in (1.3. 4) is chosen to make it agree with (1.1. 8) for $a \to 0$. Combining this equation with Poisson's equation one obtains the TFD equation

$$\nabla^2 (V - V_0 + a^2) = 4\pi e \sigma_0 \left\{ (V - V_0 + a^2)^{\frac{1}{2}} + a \right\}^3 . \qquad (1.3.\ 5)$$

As before spherical symmetry is assumed;with the substitutions

$$V - V_0 + a^2 = \frac{Ze}{r} \varphi(r) \quad , \quad r = \mu x \,, \qquad (1.3.\ 6)$$

one arrives at the <u>dimensionless TFD equation</u>

$$\frac{d^2\varphi}{dx^2} = x^{-\frac{1}{2}} \left\{ \varphi^{\frac{1}{2}} + \beta_0 x^{\frac{1}{2}} \right\}^3 \,, \qquad (1.3.\ 7)$$

where

$$\beta_0 = \left(\frac{3}{32\pi^2 Z^2} \right)^{\frac{1}{3}} \qquad (1.3.\ 8)$$

and the boundary conditions for compressed atoms are again

$$\varphi(0) = 1 \quad ; \quad \varphi(x_0) = x_0 \varphi'(x_0) \,. \qquad (1.3.\ 9)$$

For $\beta_0 \to 0$ this equation reduces to the TF equation (1.2. 3).

The TFD energy is now given instead of (1.2. 5) by

$$E = \frac{Z^2 e^2}{\mu} \left\{ \frac{1}{2}\varphi'(0) + \frac{1}{10} \int_0^{x_0} x^{-\frac{1}{2}} \left[\varphi^{\frac{1}{2}} + \beta_0 x^{\frac{1}{2}} \right]^3 \left[\varphi - 3\beta_0 x^{\frac{1}{2}} \varphi^{\frac{1}{2}} - 9\beta_0^2 x \right] dx \right\} . \qquad (1.3.10)$$

In contrast to the TF expression, (1.3.10) cannot be explicitly integrated. To find the energy one therefore has to integrate numerically or to find an analytical approximation for φ which can be used to this end. Since the constant β_0 contains the atomic number Z, it is not possible to find a universal function φ independent of Z, as in the TF case. A numerical approach then makes it necessary to solve (1.3. 7) separately for each value of Z, or at least for a range of Z-values sufficiently close to allow accurate interpolation [11]. For small values of x_0, however, we have been able to find an approximate solution [12] to (1.3. 7) valid for any β_0, by means of which (1.3.10) can be expressed explicitly in terms of x_0 and $\varphi(x_0)$.

For the pressure one has to adopt the free-electron value

$$p = \frac{2}{3} e_k \rho^{\frac{5}{3}} - \frac{1}{3} e_e \rho^{\frac{4}{3}}$$

where ρ has to be taken at the boundary $r = r_0$. In terms of the TFD function this can be expressed as

$$p v = \frac{2 Z^2 e^2}{15 \mu} x_0^{\frac{1}{2}} \left\{ \varphi^{\frac{1}{2}}(x_0) + \beta_0 x_0^{\frac{1}{2}} \left\{ \varphi^{\frac{1}{2}}(x_0) - \frac{1}{4} \beta_0 x_0^{\frac{1}{2}} \right\} \right\}. \qquad (1.3.11)$$

This again reduces to the corresponding TF expression in case $\beta_0 \to 0$.

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11) For the isolated TFD atom this has been done: see K. Umeda, J.Fac.Sci., Hokkaido Univ., Ser.II, 3 (1949) 171-244.

12) P.J. Rijnierse, Proc.Roy.Soc. A 292 (1966) 288-97.

CHAPTER 2 . PREVIOUS SOLUTIONS OF THE TF EQUATION FOR THE ISOLATED ATOM

2.1 . Approximate solutions

From the beginning it was recognized that the TF equation could not be solved by straightforward analytical methods. The non-linearity of the equation

$$\frac{d^2\varphi}{dx^2} = x^{-\frac{1}{2}}\varphi^{\frac{3}{2}} \; ; \quad \varphi(0)=1 \; , \; \varphi(\infty)=\varphi'(\infty)=0; \qquad (2.1.\ 1)$$

together with the two-point boundary conditions, posed an unsurmountable problem. There are two ways out of this dilemma: one is to solve the equation numerically, with the attendant problems of instability and the awkwardness in practice of the use of numerical tables, the other to find an approximate analytical solution, which is less accurate but easy to apply. In this section we will discuss the latter, while the numerical solutions will be treated in the following two sections.

In the analytical approximations considered to date, ease of application takes precedence over accuracy: deviations from exact values range up to 10%. Approximations for the isolated atom in the main rest on one of two basic ideas; that of Sommerfeld [1] who deduced that any solution to (2.1. 1) which vanishes as $x \to \infty$ must behave like $144\, x^{-3}$ there, and that of Brinkman [2] who argued that over a large range of x the value of $x\varphi(x)$ is nearly constant so that the right-hand side of (2.1. 1) can be written as

$$(\varphi x)^{\frac{1}{2}}\,\frac{\varphi}{x} \approx e\,\frac{\varphi}{x} \quad \text{or} \quad (\varphi x)^{-\frac{1}{2}}\varphi^2 \approx e'\,\varphi^2 \; . \qquad (2.1.\ 2)$$

Umeda and Kobayashi [3] present an extensive survey of these two families of approximate solutions.

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1) A. Sommerfeld, Z.f.Phys. 78 (1932) 283-308.
2) H.C. Brinkman, Physica 20 (1954) 44-8.
3) K. Umeda & S. Kobayashi, J.Phys.Soc.Japan 10 (1955) 749-52.

For the compressed atom a Sommerfeld type of solution was given by Sauvenier [4], and a Brinkman-like approximation by Umeda [5]. Recently, Mason [6] has derived a rational approximation of the Chebyshev type for this case.

Whereas these approximate analytical solutions are very valuable when the TF potential is invoked to solve e.g. a Schrödinger equation, their inaccuracy makes them useless as soon as the boundary values are required, as in the equation of state (1.2.15) or the energy (1.2.14). Therefore we will now discuss the more accurate numerical solutions.

2.2 . Numerical solutions: "outward" integration

The first numerical values for the TF function were given by the originators of the statistical model; Thomas' solution [7] is very limited in range and rather inaccurate, while Fermi [8] does not indicate how he obtained his values, which are slightly better.

Following this pioneering work, a number of investigators have solved (2.1. 1) numerically, starting the integration from $x = 0$ with the help of a series expansion due to Baker [9]:

$$\varphi(x) = 1 + Bx + \frac{4}{3}x^{\frac{3}{2}} + \frac{2}{5}Bx^{\frac{5}{2}} + \frac{1}{3}x^3 + \frac{3}{70}B^2x^{\frac{7}{2}} + \frac{2}{15}Bx^4 + \left(\frac{2}{27} - \frac{1}{252}B^3\right)x^{\frac{9}{2}} + \ldots \quad . \qquad (2.2.\ 1)$$

Generating starting values from this expansion, Baker [9], Slater and Krutter [10] and Feynman et.al. [11] integrated the TF equation numerically, for increasing values of x . Taking various trial

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4) H. Sauvenier, Bull.Soc.Roy.Sci., Liège 8 (1939) 313.

5) K. Umeda, J.Phys.Soc.Japan 9 (1954) 291-2.

6) J.C. Mason, Proc.Phys.Soc. 89 (1966) 772-4.

7) L.H. Thomas, Proc.Camb.Phil.Soc. 23 (1927) 542-8.

8) E. Fermi, Z.f.Phys. 48 (1928) 73-9.

9) E.B. Baker, Phys.Rev. 36 (1930) 630-47. The last term quoted by Baker contains an error (corrected here).

10) J.C. Slater & H.M. Krutter, Phys.Rev. 47 (1935) 559-68.

11) R.P. Feynman, N. Metropolis & E. Teller, Phys.Rev. 75 (1949) 1561-73.

values for the initial slope $\mathcal{B}$ they tried to satisfy the second boundary condition $\varphi(\infty) = 0$. The main drawback of this method is that the solutions thus obtained for large x are very sensitive to very small changes in $\mathcal{B}$; any value just below the isolated-atom value $\mathcal{B}_0$ leads to a solution which vanishes at a finite x -value, while any value just above $\mathcal{B}_0$ yields a solution which becomes infinitely large. Accompanying this, errors tend to accumulate very quickly because of this instability. A different method was therefore adopted by Miranda [12] who was able to construct upper and lower bounds for $\mathcal{B}_0$. He obtained these by a procedure of outward integration, and then for large x fitted the calculated values of φ to an asymptotic formula. His final result is $\mathcal{B}_0 = -1.5880464$, for which he claims an accuracy of 1 in 10^6; comparison with the more accurate value $\mathcal{B}_0 = -1.5880710226$ (see chapter 3) however shows a relative error exceeding 1 in 10^5.

2.3 . Numerical solutions: "inward" integration

In the previous paragraph we saw that instability is inherent to integration with increasing x . Therefore it is plausible to try to integrate from the large- x side. Lacking a suitable approximation to generate starting values, Bush and Caldwell [13] assumed trial values of $\varphi(10)$, fixing $\varphi'(10)$ by requiring that $\varphi(\infty) = 0$, and then worked backwards; at $x = 0.2$ they joined this solution to values obtained from Bakers series (2.2. 1). Thus they obtained the first reliable 3-figure table of the TF function.

A much more accurate procedure became possible when Coulson and March [14] gave their asymptotic solution of the Sommerfeld type

$$\varphi(x) = 144\, x^{-3} \sum_{k=0}^{\infty} c_k \left(F\, x^{\lambda_-}\right)^k . \qquad (2.3.\ 1)$$

Here the value of $\lambda_- = \frac{7 - \sqrt{73}}{2} = -0.77200\ldots$, F was given by CM as 13.21 and the coefficients c_k can be found in table 2.1 below.

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12) C. Miranda, Mem.Reale Accad.d'Ital. 5 (1934) 285-322.

13) V. Bush & S.H. Caldwell, Phys.Rev. 38 (1931) 1898-902.

14) C.A. Coulson & N.H. March, Proc.Phys.Soc. A63 (1950) 367-74. (Hereafter referred to as CM).

Table 2.1 . The coefficients c_k of Coulson and March's solution.

$c_0 = 1.0000$	$c_3 = -0.3134$	$c_6 = 0.0207$
$c_1 = -1.0000$	$c_4 = 0.1374$	$c_7 = -0.0074$
$c_2 = 0.6257$	$c_5 = -0.0551$	$c_8 = 0.0026$

Kobayashi et.al.[15] started from this expression and, proceeding by numerical integration, obtained a solution which remains finite for $x = 0$. They could fit the boundary condition $\varphi(0) = 1$ by invoking Sommerfeld's [1] invariance theorem: if $\varphi(x)$ satisfies the TF equation (2.1. 1) then so does $e^3 \varphi(ex)$. Thus the solution which satisfies $\varphi(0) = 1$ may be found by a simple scale transformation.

Taking the trial value $F = 13$ in (2.3. 1) KNMU integrate inwards, taking $x^{\frac{1}{2}}$ as the independent variable for $x = 1$ in order to avoid the singularity at $x = 0$. There they find a value $\varphi(0) \neq 1$. If we indicate the KMNU solution with $F = 13$ by $\varphi_{13}(x)$ and if $\varphi_{13}(0) = a$, then by the invariance property the true TF function $\varphi(x)$ can be written as

$$\varphi(x) = a^{-1} \varphi_{13}(a^{-\frac{1}{3}} x) \quad . \tag{2.3. 2}$$

Hence

$$B_0 \equiv \varphi'(x)\Big|_{x=0} = a^{-\frac{4}{3}} \varphi_{13}'(y)\Big|_{y=0} \quad , \tag{2.3. 3}$$

and from (2.3. 1) we have for large x with (2.3. 2)

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15) S. Kobayashi, T. Matsukuma, S. Nagai & K. Umeda, J.Phys.Soc. Japan 10 (1955) 759-62. (Referred to as KMNU). The values of the coefficients c_k of (2.3. 1) given in their table II are in error beyond c_{10} .

$$\varphi(x) = 144\, x^{-3} \sum_{k=0}^{\infty} e_k \left(F x^{\lambda_-}\right)^k$$

$$= a^{-1} \varphi_{13}(a^{-\frac{1}{3}} x) = 144\, x^{-3} \sum_{k=0}^{\infty} e_k \left\{13 (a^{-\frac{1}{3}} x)^{\lambda_-}\right\}^k . \qquad (2.3.4)$$

so that

$$F = 13\, a^{-\frac{1}{3}\lambda_-} . \qquad (2.3.5)$$

For $x = 0$ KMNU obtain the values

$$a = \varphi_{13}(0) = 1.0834\ 68762 \quad ; \quad \varphi_{13}'(0) = -1.7672\ 24730, \qquad (2.3.6)$$

and we calculate [+)] with the help of (2.3.3-5)

$$B_0 = -1.588071021 \quad ; \quad F = 13.27097383 . \qquad (2.3.7)$$

[+)] The values (2.3.6) were taken from the KMNU paper, and B_0 and F in (2.3.7) calculated from them. (The values of B_0 and F actually quoted in the original paper seem to have been affected by an error in the very last stage of their calculation. The recalculated values quoted here agree very well with the more accurate derivations in chapter 3 of this thesis.)

CHAPTER 3 . ALGEBRAIC SOLUTION OF THE TF EQUATION - SUMMARY OF RESULTS DERIVED IN THIS THESIS

In this chapter we will give in condensed form the complete solution of the TF equation for isolated and for moderately compressed atoms. The detailed discussion of the various aspects is given in the chapters following this one; here we give only the most important results, enabling the reader to sample the currants without first having to eat the cake.

3.1 . Motivation and outline of the approach adopted

In the previous chapter it already became clear that numerical integration, as a method of solving the TF equation, is severely limited. We noticed the instability of the solutions obtained, with the attendant accumulation of errors and the difficulty of assessing their total magnitude. Even graver is the objection that solutions thus obtained are not amenable to generalization, making it necessary to repeat the entire numerical integration for each different atom size and for each change in the type of boundary condition. For this reason, too, they form a poor starting point for other generalizations, e.g. to higher temperatures.

The essence of the approach adopted in this thesis can be stated succinctly as follows. It is relatively simple to establish power series expansions for solutions to the TF equation, converging in limited regions around the boundary points. On the other hand, by careful examination of the structure of a series it often proves possible to convert it into a form which converges very much faster and over a wider region than the original. In this thesis we have achieved this for the Baker series, convergent near the origin, and for the Coulson-March (CM) and the Coulson-March-Gilvarry (CMG) series, convergent for large values of the independent variable. In fact, we have succeeded to such an extent that the replacement series overlap: thereby these series could be matched with extremely high precision - 11 significant figures - transcending in accuracy the values obtained to date by numerical integration.

Our success in the detailed investigation of the important TF series also raises hopes in a wider context. The elucidation of the structure of series expansions is of increasing importance, both in its own right - cf. the growing interest in Ising model series and perturbation expansions - and as a tool in solving many non-linear equations important in physics and applied mathematics - e.g. those in astrophysics, fluid dynamics and general relativity. In the latter case, the major hope of solving these equations lies in constructing series solutions and matching them (see e.g. the book by Van Dyke [1a] for a number of examples). This makes our success with the TF equation the more encouraging.

A brief survey of a few problems which might be treated by similar techniques is presented in chapter 9.

3.2. Expansion near the origin: Baker series

The starting point is the series found by Baker [1]:

$$\varphi(x) = 1 + Bx + \frac{4}{3}x^{\frac{3}{2}} + \frac{2}{5}Bx^{\frac{5}{2}} + \frac{1}{3}x^{3} + \frac{3}{70}B^{2}x^{\frac{7}{2}} + \frac{2}{15}Bx^{4} + \left(\frac{2}{27} - \frac{1}{252}B^{3}\right)x^{\frac{9}{2}} + \dots \quad . \qquad (3.2.1)$$

We can write this formally as

$$\varphi(x) = \sum_{l=0}^{\infty}\sum_{s=0}^{\infty} a_{l,s}\, x^{\frac{3}{2}l}\,(xB)^{s} \quad . \qquad (3.2.2)$$

The properties of the series (3.2.2) are extensively discussed in chapter 4; in accordance with our program we just quote here the main results of this analysis.

For arbitrary, but fixed x, $\varphi(x)$ may be written as

$$\varphi(x) = \sum_{s=0}^{\infty} b_s\, B^{s} \quad , \quad b_s = x^{s}\sum_{l=0}^{\infty} a_{l,s}\, x^{\frac{3}{2}l} \; ; \qquad (3.2.3)$$

1a) M. Van Dyke, Perturbation Methods in Fluid Mechanics, Academic Press, New York/London (1964).

1) E.B. Baker, Phys.Rev. 36 (1930) 630-47.

Table 3.1

The coefficients b_s and b_s' of (3.2. 3/4) for $\varkappa = 1$

s	b_s	b_s'
0	.275265795622429E+01	.340817359517940E+01
1	.156024254598906E+01	.269119641452955E+01
2	.538498616410652E-01	.213214851710480E-00
3	-.233823354965220E-02	-.868716112626928E-02
4	.383645053446426E-03	.171773672950269E-02
5	-.828882836999236E-04	-.413722253440842E-03
6	.213479629450280E-04	.116742997399620E-03
7	-.616595639248696E-05	-.365161339347970E-04
8	.193160161209048E-05	.122836700621610E-04
9	-.643043780785505E-06	-.436237835305871E-05
10	.224455824094235E-06	.161580589920314E-05
11	-.813819697248948E-07	-.618960987297413E-06
12	.304430458240800E-07	.243723614226041E-06
13	-.116897086120565E-07	-.982003945305465E-07
14	.458961096886433E-08	.403451029975301E-07
15	-.183682263326616E-08	-.168553445669609E-07
16	.747489498180147E-09	.714495463822337E-08
17	-.308684924176450E-09	-.306761371674311E-08
18	.129144538132890E-09	.133199264077437E-08
19	-.546616981573405E-10	-.584210626811702E-09
20	.233790226558628E-10	.258555423332519E-09
21	-.100941657677941E-10	-.115364289892650E-09
22	.439583006426465E-11	.518553801719325E-10
23	-.192935955949793E-11	-.234658561387859E-10
24	.852911595956776E-12	.106844280534431E-10
25	-.379546267507360E-12	-.489239111831571E-11

and similarly

$$x\,\varphi'(x) = \sum_{s=0}^{\infty} b_s'\,B^s \quad , \quad b_s' = x^s \sum_{l=0}^{\infty} \left(\tfrac{3}{2}l+s\right) a_{l,s}\, x^{\frac{3}{2}l} \qquad (3.2.\ 4)$$

With this formulation we can - for fixed x - calculate the coefficients b_s and b_s' once and for all; for any value of the initial slope B we can then find φ and φ' by a simple summation. Since we have chosen $x=1$ as the point to join this expansion to one valid for $x\to\infty$ we have calculated the values of $b_s(x=1)$ and $b_s'(x=1)$ and collected these in table 3.1 .

The expressions (3.2. 3/4) are not particularly convenient for calculating $\varphi(x)$ as a function of x . For this purpose it is preferable to rewrite (3.2. 2) as

$$\varphi(x) = \sum_{k=0}^{\infty} a_k\, x^{\frac{1}{2}k} \quad , \quad a_k = \sum_{3l+2s=k} a_{l,s}\, B^l . \qquad (3.2.\ 5)$$

The coefficients a_k have been evaluated for the isolated-atom value $B_0 = -1.5880710226$; these values are given in table 3.2 . The series (3.2. 5) converges for $x \lesssim 0.44$, but it converges too slowly for direct numerical calculation as it stands. However, highly accurate values may be extracted from the series by converting it into $(n, n+2)$ Padé approximants. These rational approximations, of the form

$$(n, n+2) = \frac{\sum_{i=0}^{n+2} p_i\, x^{\frac{1}{2}i}}{\sum_{i=0}^{n} q_i\, x^{\frac{1}{2}i}} \qquad (3.2.\ 6)$$

have been calculated for $n = 12$; the values of p_i and q_i , and of the corresponding coefficients p_i' and q_i' for φ', are tabulated in table 3.3 . These Padé approximants yield at least 12-figure accuracy right up to $x = 1$, and at least 9-figure accuracy up to $x = 2$.

Table 3.2

The coefficients a_k (3.25) for the isolated atom

k	a_k	k	a_k
0	.100000000000000E+01	21	.183630138770471E-01
1	.000000000000000E-99	22	-.215554971245295E-01
2	-.158807102260000E+01	23	.257019114152481E-01
3	.133333333333333E+01	24	-.309897649249270E-01
4	.000000000000000E-99	25	.377325337147117E-01
5	-.635228409040000E-00	26	-.463731187493039E-01
6	.333333333333333E-00	27	.574928598343257E-01
7	.108084410263792E-00	28	-.718526562912179E-01
8	-.211742803013333E-00	29	.904603152141467E-01
9	.899671962902535E-01	30	-.114659258089710E-00
10	.144112547018389E-01	31	.146244556793361E-00
11	-.271286107057753E-01	32	-.187619238525825E-00
12	-.295055008478292E-03	33	.242007418156681E-00
13	.173443041642727E-01	34	-.313745267564561E-00
14	-.167709556143035E-01	35	.408678305314600E-00
15	.112763141431646E-01	36	-.534704559574435E-00
16	-.911028066991997E-02	37	.702518484493754E-00
17	.102762683449552E-01	38	-.926631598151114E-00
18	-.123240451261030E-01	39	.122677504660947E+01
19	.141442924276242E-01	40	-.162983Q00387084E+01
20	-.159860960349775E-01		

Table 3.3

The coefficients p_i, q_i and p_i', q_i' of the Padé approximants (3.2.6) for the isolated atom

i	p_i	q_i	i	p_i'	q_i'
0	.100000000000E+01	.100000000000E+01	0	-.158807102260E+01	.100000000000E+01
1	.591878461927E+01	.591878461927E+01	1	-.753436504050E+01	.600373969729E+01
2	.140238736359E+02	.156119446585E+02	2	-.134760211599E+02	.160468267425E+02
3	.167922510200E+02	.248583680295E+02	3	-.108079739632E+02	.260149299607E+02
4	.103979341597E+02	.272990982527E+02	4	-.320190319985E+01	.294051068348E+02
5	.286751478789E+01	.221636709224E+02	5	.182929436660E-00	.248892009546E+02
6	.119036061050E-00	.137538990370E+02	6	.329304455833E-01	.163109568312E+02
7	-.166864011182E-01	.661813762569E+01	7	-.462057604017E-01	.842276581153E+01
8	.171357475948E-01	.246651750606E+01	8	.238647367678E-01	.343420943068E+01
9	-.447489604142E-02	.697990734232E-00	9	-.618828787336E-02	.108985488364E+01
10	-.215689510166E-03	.143906950187E-00	10	-.342652292934E-03	.262053483135E-00
11	.534159211608E-03	.195223041317E-01	11	.959084681508E-03	.435372640964E-01
12	-.185529744748E-03	.136899271638E-02	12	-.384754565484E-03	.439847795829E-02
13	.324444635580E-04		13	.773372959345E-04	
14	-.252855166543E-05		14	-.687389195009E-05	

3.3 . **Expansion near infinity for the isolated atom: Coulson-March series**

In this region we start from the series obtained by Coulson and March [2]:

$$\varphi(x) = 144\, x^{-3} \sum_{k=0}^{\infty} c_k \left(F x^{\lambda_-}\right)^k \quad , \qquad (3.3.\ 1)$$

valid for large positive x . A detailed account of its derivation and of the elucidation of its structure will be found in chapter 5. The coefficients c_k are collected in table 3.4 for $0 \leq k \leq 30$, the value of $\lambda_- = \frac{7 - \sqrt{73}}{2} = -0.7720018726...$ (3.3. 2)

For the isolated-atom value $F = 13.270973848$ the series (3.3. 1) converges for $x \gtrsim 4.75$; near this limit the convergence is so slow that accurate summation is possible only for $x \gtrsim 10$.

Analysing the series (3.3. 1) we realize that its main singularity is a fourth-order pole: writing φ in the form

$$\varphi(x) = 144\, x^{-3} \left\{ \sum_{k=0}^{\infty} \delta_k \left(F x^{\lambda_-}\right)^k \right\}^{-4} \quad , \qquad (3.3.\ 3)$$

numerically much better convergence is achieved. Some of the coefficients δ_k are given in table 3.5 ; they give 6-figure accuracy for $x \gtrsim 2.5$. In appendix 10.12 we will calculate from (3.3. 3) March's [3] "master solutions", defined by putting $F = \pm 1$ in (3.3. 1).

Still faster convergence over a wider range is obtained by introducing a new independent variable

$$u = \frac{\beta F x^{\lambda_-}}{1 + \beta F x^{\lambda_-}} \quad , \qquad (3.3.\ 4)$$

where

$$\beta = 0.2507623787.... \quad . \qquad (3.3.\ 5)$$

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2) C.A. Coulson and N.H. March, Proc.Phys.Soc. A 63 (1950) 367-74.

3) N.H. March, Proc.Camb.Phil.Soc. 48 (1952) 665-82.

Table 3.4

The coefficients c_k of the C.M. series (3.3.1)

k	c_k	k	c_k
0	.100000000000000E+01	16	.234263216206774E-06
1	-.100000000000000E+01	17	-.691031290629697E-07
2	.625697497782349E-00	18	.202144402461023E-07
3	-.313386115073309E-00	19	-.586883726659920E-08
4	.137391276719371E-00	20	.169228967471091E-08
5	-.550834346641491E-01	21	-.484947296184278E-09
6	.207072584991917E-01	22	.138179140746420E-09
7	-.741452947849571E-02	23	-.391670654111897E-10
8	.255553116794870E-02	24	.110486378825038E-10
9	-.854165377806924E-03	25	-.310287206325100E-11
10	.278373839349473E-03	26	.867815397770538E-12
11	-.888226094136591E-04	27	-.241782703567386E-12
12	.278359915878395E-04	28	.671228958979403E-13
13	-.858949083219027E-05	29	-.185723018657859E-13
14	.261505871330370E-05	30	.512274393418862E-14
15	-.786798261946265E-06		

Table 3.5

The coefficients δ_k of the modified CM series (3.3.3)

k	δ_k	k	δ_k
0	.100000000000000E+01	16	-.723226792382381E-19
1	.250000000000000E-00	17	.100731833242623E-19
2	-.174374445587235E-03	18	-.144323922981419E-20
3	.356071134331017E-05	19	.212144750255850E-21
4	-.128731807439271E-06	20	-.319191567680414E-22
5	.643080048407153E-08	21	.490602313745848E-23
6	-.400418712444300E-09	22	-.768970101043208E-24
7	.293424608556416E-10	23	.122722605698767E-24
8	-.243976914655237E-11	24	-.199152256762286E-25
9	.224489539711181E-12	25	.328221446728015E-26
10	-.224494830691307E-13	26	-.548783504869067E-27
11	.240730157157307E-14	27	.929965585265983E-28
12	-.273952206345821E-15	28	-.159582558097920E-28
13	.328174989750201E-16	29	.277085567858257E-29
14	-.411139332557944E-17	30	-.486453415820861E-30
15	.535815727293826E-18		

Table 3.6

The coefficients γ_k and γ_k' for φ and φ' (3.3.6)

k	γ_k	k	γ_k'
0	.100000000000000E+01	0	-.300000000000000E+01
1	-.398783902560817E+01	1	.150421362724557E+02
2	.596254074289271E+01	2	-.301724266629440E+02
3	-.396141458214374E+01	3	.302650874124441E+02
4	.986680663825830E-00	4	-.151815776996146E+02
5	.862058263143250E-05	5	.304681814348137E+01
6	.591640202813770E-05	6	-.118785170807821E-04
7	.416991735142858E-05	7	-.763919941248515E-05
8	.300756004562153E-05	8	-.506312800674662E-05
9	.221347401708370E-05	9	-.344494092885428E-05
10	.165837776970438E-05	10	-.239858597055639E-05
11	.126237241361949E-05	11	-.170450234336115E-05
12	.974691072436120E-06	12	-.123354067514480E-05
13	.762271871914467E-06	13	-.907434681239750E-06
14	.603102538119691E-06	14	-.677476594320325E-06
15	.482232976330658E-06	15	-.512622297096967E-06
16	.389324832627409E-06	16	-.392655083880782E-06
17	.317110611067095E-06	17	-.304149590350531E-06
18	.260404305817061E-06	18	-.238030173832402E-06
19	.215453933806986E-06	19	-.188060757158901E-06
20	.179510353574526E-06	20	-.149891676103877E-06
21	.150535470594452E-06	21	-.120446798570119E-06
22	.127001819993084E-06	22	-.975226338151750E-07
23	.107753007570439E-06	23	-.795219231320334E-07
24	.919052812715845E-07	24	-.652739823213709E-07
25	.787772814448378E-07	25	-.539118823205984E-07
26	.678393432826137E-07	26	-.447874112953894E-07
27	.586765276974948E-07	27	-.374114918020571E-07
28	.509613992461448E-07	28	-.314119658591504E-07
29	.444337969192915E-07	29	-.265033710204385E-07
30	.388856713126629E-07	30	-.224650876271209E-07

In terms of u the TF function is written as

$$\varphi(x) = 144\, x^{-3} \sum_{k=0}^{\infty} \gamma_k\, u^k \quad ; \quad \varphi'(x) = 144\, x^{-4} \sum_{k=0}^{\infty} \gamma_k'\, u^k \quad . \qquad (3.3.\ 6)$$

With the help of the coefficients γ_k and γ_k', listed in table 3.6, φ can be calculated to 12 significant figures for $x \gtrsim 1$, to 6 figures for $x \gtrsim 0.6$.

It is convenient at this stage to introduce instead of F as a parameter

$$u_1 \equiv u(x=1) = \frac{\beta F}{1+\beta F} \quad ; \quad F = \frac{u_1}{\beta\,(1-u_1)} \quad . \qquad (3.3.\ 7)$$

The definition (3.3. 4) of u may thus be rewritten as

$$u = \frac{u_1\, x^{\lambda}}{1 - u_1 + u_1\, x^{\lambda}} \quad . \qquad (3.3.\ 8)$$

3.4 . Joining expansions for the isolated atom

We have now two different expressions for the function values at $x = 1$: the Baker-type forms (3.2. 3/4)

$$\varphi(1) = \sum_{s=0}^{\infty} b_s(x=1)\, B_0^{\,s} \quad , \quad \varphi'(1) = \sum_{s=0}^{\infty} b_s'(x=1)\, B_0^{\,s} \qquad (3.4.\ 1)$$

and the CM-type forms (3.3. 6)

$$\varphi(1) = 144 \sum_{k=0}^{\infty} \gamma_k\, u_1^{\,k} \quad , \quad \varphi'(1) = 144 \sum_{k=0}^{\infty} \gamma_k'\, u_1^{\,k} \quad . \qquad (3.4.\ 2)$$

The parameters B_0 and u_1 are determined by the continuity of φ and φ' . The resulting non-algebraic equations are conveniently solved by means of Newton's method of successive approximations, generalized to two variables. A suitable form of this method is given in appendix 10.32.

Starting with approximate values $B_0 = -1.5$ and $u_1 = 0.75$, we find after 6 iterations

$$\left.\begin{aligned} B_0 &= -1.5880710226 \quad ; \quad u_1 = 0.76893897310 \\ &\qquad\qquad\quad\;\; F = 13.270973848 \quad . \end{aligned}\right\} \qquad (3.4.\ 3)$$

and hence

In order to reach the accuracy of (3.4. 3) we had to employ convergence-improving techniques, discussed in appendix 10.2 . The values given here agree almost perfectly with the recalculated KMNU values (2.3. 7) to the limit of accuracy expected by those authors. We believe that our calculations are accurate to at least 2 or 3 units in the last figure quoted.

3.5 . <u>Expansions near the boundary for the compressed atom: Coulson-March-Gilvarry series</u>

To treat the compressed atom we introduce a generalization of the CM series due to Gilvarry and March [4] (hereafter called the Coulson-March-Gilvarry (CMG) solution):

$$\varphi(x) = 144\, x^{-3} \sum_{k=0}^{\infty} \sum_{\ell=0}^{\infty} c_{k,\ell} \left(F_- x^{\lambda_-}\right)^k \left(F_+ x^{\lambda_+}\right)^\ell , \qquad (3.5.\ 1)$$

where, as in section 3.2 , $\lambda_- = \frac{7-\sqrt{73}}{2} = -.7720018726...$ and $\lambda_+ = \frac{7+\sqrt{73}}{2} = 7.7720018726..$ (3.5. 2)

The parameters F_- and F_+ depend on the value of the boundary radius x_0 and for $x_0 \to \infty$ they approach the values $F_- \to 13.270973848$, corresponding to F of section 3.3 , and $F_+ \to 0.9636517351... \cdot x_0^{-\lambda_+}$. (3.5. 3)

The coefficients $c_{k,\ell}$ up to $k, \ell = 8$ are listed in table 3.7 .

The CMG series is analysed in chapter 6; quoting again only results, we are led to write $\varphi(x)$ in terms of new independent variables defined by

$$u = \frac{\beta F_- x^{\lambda_-}}{1+\beta F_- x^{\lambda_-}} , \quad v = F_+ x^{\lambda_+} \left(1+\beta F_- x^{\lambda_-}\right)^{\kappa} , \qquad (3.5.\ 4)$$

with

$$\beta = 0.2507623787 ... \qquad (3.5.\ 5)$$

as in (3.3. 5).

Thus we write

$$\varphi(x) = 144\, x^{-3} \sum_{k=0}^{\infty} \sum_{\ell=0}^{\infty} \gamma_{k,\ell}\, u^k v^\ell . \qquad (3.5.\ 6)$$

---

4) J.J. Gilvarry & N.H. March, Phys.Rev. <u>112</u> (1958) 140-9.

Table 3.7

The coefficients $c_{k,l}$ of the CMG series (3.5.1)

k \ l	0	1	2	l \ k
0	.1000000000E+01	.1000000000E+01	.3548671274E-01	0
1	-.1000000000E+01	.1500000000E+01	.1418150859E-00	1
2	.6256974978E-00	.9362229806E-00	.2654819794E-00	2
3	-.3133861151E-00	.3108640080E-00	.3089792585E-00	3
4	.1373912767E-00	.5774411092E-01	.2501643335E-00	4
5	-.5508343466E-01	.5632267301E-02	.1493523331E-00	5
6	.2070725850E-01	.2112721232E-03	.6797390158E-01	6
7	-.7414529478E-02	-.2635803348E-05	.2403476507E-01	7
8	.2555531168E-02	-.1945414574E-06	.6661503657E-02	8

k \ l	3	4	5	l \ k
0	-.1150085184E-02	.2648199477E-03	-.8029682396E-04	0
1	-.7474949605E-02	.2382834305E-02	-.9232500688E-03	1
2	-.2335131666E-01	.1042041145E-01	-.5191568000E-02	2
3	-.4667332147E-01	.2950525749E-01	-.1902634139E-01	3
4	-.6702888995E-01	.6080014309E-01	-.5109898959E-01	4
5	-.7363420861E-01	.9716712107E-01	-.1072154714E-00	5
6	-.6431769791E-01	.1253244100E-00	-.1829644190E-00	6
7	-.4583936855E-01	.1340360745E-00	-.2610409117E-00	7
8	-.2714217271E-01	.1212085063E-00	-.3176570284E-00	8

k \ l	6	7	8	l \ k
0	.3085197073E-04	-.1384863727E-04	.6942066368E-05	0
1	.4318669944E-03	-.2284767664E-03	.1318871953E-03	1
2	.2968304019E-02	-.1855974068E-02	.1236220565E-02	2
3	.1335211201E-01	-.9895330882E-02	.7621292439E-02	3
4	.4420535583E-01	-.3894586815E-01	.3475938466E-01	4
5	.1148559519E-00	-.1206651466E-00	.1250753397E-00	5
6	.2438652305E-00	-.3064818256E-00	.3698030416E-00	6
7	.4350378802E-00	-.6562129972E-00	.9238780578E-00	7
8	.6653671671E-00	-.1208740828E+01	.1990527572E+01	8

Table 3.8

The coefficients $\gamma_{k,\ell}$ of the modified CMG series (3.5.6)

k \ ℓ	0	1	2	ℓ / k
0	.1000000000E+01	.1000000000E+01	.3548671274E-01	0
1	-.3987839026E+01	-.4018241462E+01	-.1441985209E-00	1
2	.5962540743E+01	.6052796232E+01	.2192192514E-00	2
3	-.3961414582E+01	-.4051289251E+01	-.1479911199E-00	3
4	.9866806638E-00	.1016554064E+01	.3734695128E-01	4
5	.8620582631E-05	-.1139144916E-03	-.1387233985E-03	5
6	.5916402028E-05	-.2252141764E-03	-.3472274085E-03	6
7	.4169917351E-05	-.4980150664E-03	-.1037962904E-02	7
8	.3007560046E-05	-.1296753074E-02	-.4094314798E-02	8

k \ ℓ	3	4	5	ℓ / k
0	-.1150085184E-02	.2648199477E-03	-.8029682396E-04	0
1	.4693659762E-02	-.1090438275E-02	.3330685429E-03	1
2	-.7181800058E-02	.1681878902E-02	-.5175288283E-03	2
3	.4879531222E-02	-.1151940443E-02	.3571312884E-03	3
4	-.1245792551E-02	.2958027605E-03	-.9240952873E-04	4
5	-.5992362473E-05	.2153310793E-06	-.5671836483E-07	5
6	-.1679204601E-04	.6741907583E-06	-.1872717000E-06	6
7	-.5573919158E-04	.2402872276E-05	-.6894005140E-06	7
8	-.2424558012E-03	.1099211131E-04	-.3234506977E-05	8

k \ ℓ	6	7	8	ℓ / k
0	.3085197073E-04	-.1384863727E-04	.6942066368E-05	0
1	-.1289021894E-03	.5827604359E-04	-.2942040501E-04	1
2	.2017645102E-03	-.9188393540E-04	.4672495628E-04	2
3	-.1402788365E-03	.6436344397E-04	-.3297630497E-04	3
4	.3657856510E-04	-.1691423952E-04	.8734176739E-05	4
5	.1888282415E-07	-.7789747674E-08	.3674809377E-08	5
6	.6595871683E-07	-.2873017614E-07	.1434529793E-07	6
7	.2494022114E-06	-.1109905382E-06	.5646583789E-07	7
8	.1191590748E-05	-.5375594450E-06	.2765041909E-06	8

This expression converges much faster than (3.5. 1), as can be seen by comparing the old coefficients $c_{k,\ell}$ with the new $\gamma_{k,\ell}$ tabulated in table 3.8 . For convenience new parameters are introduced to replace F_- and F_+ :

$$u_1 \equiv u(x=1) = \frac{\beta F_-}{1+\beta F_-} \quad , \quad F_- = \frac{u_1}{\beta(1-u_1)} \quad ,$$

and (3.5. 7)

$$v_0 \equiv v(x=x_0) = F_+ x_0^{\lambda_+}(1+\beta F_- x_0^{\lambda_-})^{10} \quad , \quad F_+ = v_0 x_0^{-\lambda_+}\left[\frac{1-u_1}{1-u_1+u_1 x_0^{\lambda_-}}\right]^{10} .$$

Finally we express the independent variables u and v as

$$u = \frac{u_1 x^{\lambda_-}}{1-u_1+u_1 x^{\lambda_-}} \quad , \quad v = v_0 \left(\frac{x}{x_0}\right)^{\lambda_+}\left[\frac{1-u_1+u_1 x^{\lambda_-}}{1-u_1+u_1 x_0^{\lambda_-}}\right]^{10} . \quad (3.5. 8)$$

3.6 . Joining expansions for the compressed atom

To determine the parameters B , u_1 and v_0 for the compressed atom one has to match

$$\left.\begin{aligned} \varphi_{Baker}(1) &= \sum_{s=0}^{\infty} b_s(x=1) B^s \quad , \quad \varphi'_{Baker}(1) = \sum_{s=0}^{\infty} b'_s(x=1) B^s , \\ \varphi_{emg}(1) &= 144 \sum_{k,\ell=0}^{\infty} \gamma_{k,\ell}\, u_1^k v_1^\ell \quad , \quad \varphi'_{emg}(1) = 144 \sum_{k,\ell=0}^{\infty} \gamma'_{k,\ell}\, u_1^k v_1^\ell , \end{aligned}\right\} \quad (3.6. 1)$$

with

and at the same time introduce the boundary condition at $x = x_0$, i.e.

$$\varphi_{emg}(x_0) = x_0 \varphi'_{emg}(x_0) \quad , \text{ or } \sum_{k,\ell=0}^{\infty} \gamma_{k,\ell}\, u_0^k v_0^\ell = \sum_{k,\ell=0}^{\infty} \gamma'_{k,\ell}\, u_0^k v_0^\ell . \quad (3.6. 2)$$

We have introduced, in obvious notation, the coefficients $\gamma'_{k,\ell}$ of the expansion for φ'_{emg} in terms of u and v , and the parameters

$$\left.\begin{aligned} v_1 &\equiv v(x=1) = v_0 x_0^{-\lambda_+}(1-u_1+u_1 x_0^{\lambda_-})^{-10} \quad , \\ u_0 &\equiv u(x=x_0) = u_1 x_0^{\lambda_-}(1-u_1+u_1 x_0^{\lambda_-})^{-1} \quad . \end{aligned}\right\} \quad (3.6. 3)$$

Table 3.9

The coefficients τ_i and $\mathcal{B}_i$ of the expansions (3.6.4)

i	τ_i	$\mathcal{B}_i$
0	.7689389731E-00	-.1588071023E+01
1	-.4615309945E-02	.2624540616E-00
2	-.5045151507E-04	.1469698820E-01
3	.4217750647E-05	.2417727497E-03
4	.8813596704E-07	-.2365163421E-04
5	-.1651703935E-07	-.1460264258E-05

Table 3.10

The coefficients σ_i of (3.6.6) and π_i of (3.6.8), and the expansion coefficients of $(1-u_0)^{-4}\,\psi^0(u_0)$

i	σ_i	π_i	Expansion of $(1-u_0)^{-4}\psi^0(u_0)$
0	.9636517351E-00	.1995755466E+01	.1995755466E+01
1	.4203625905E-00	-.7542404436E+01	.4406174294E-00
2	.4981711467E-00	.1072880232E+02	.5167392360E-00
3	.5869243350E-00	-.6803359970E+01	.6029142625E-00
4	.6879323781E-00	.1621727322E+01	.6996632075E-00
5	.8026600710E-00	-.3975018821E-03	.8071092677E-00
6	.9328943478E-00	-.7899231255E-03	.9245857166E-00
7	.1081355771E+01	-.1641909821E-02	.1049783918E+01
8	.1254553532E+01	-.3829829913E-02	.1176565406E+01
9	.1484836755E+01	-.1121520791E-01	.1287576506E+01
10	.4120799182E+01	-.5350672604E-01	.1311956818E+01
11	-.5674372011E-00	-.3355497823E+01	-.2176651882E+01
12	.1410076750E+01	.1222033262E+02	-.3842751993E-00
13	.1388157424E+01	-.1624217615E+02	-.7591148953E-00
14	.1329861076E+01	.9524735625E+01	-.1224637104E+01
15	.1227965866E+01	-.2092891944E+01	-.1797199904E+01

The requirement that $\varphi(1)$ and $\varphi'(1)$ must be the same for either set of equations (3.6. 1) enables us to write $\mathcal{B}$ and u, as power series in v, :

$$\mathcal{B} = \sum_{i=0}^{\infty} \mathcal{B}_i \, v_1^{\,i} \quad , \quad u_1 = \sum_{i=0}^{\infty} \tau_i \, v_1^{\,i} \quad . \qquad (3.6.\ 4)$$

This is achieved by substituting these expressions into (3.6. 1) and requiring that function and derivative be continuous to any order of the expansion variable v, . We choose for $\mathcal{B}_0$ and τ_0 the isolated-atom values

$$\mathcal{B}_0 = -1.5880710226 \quad , \quad \tau_0 = 0.76893897310 \quad , \qquad (3.6.\ 5)$$

so that the zero-order equations are automatically satisfied. The resultant values of $\mathcal{B}_i$ and τ_i are given in table 3.9 . The boundary condition (3.6. 2) enables us to write v_0 as a power series

$$v_0 = \sum_{i=0}^{\infty} \sigma_i \, u_0^{\,i} \quad , \qquad (3.6.\ 6)$$

again substituting and expanding to any order in the variable u_0. Here the zero-order equation is easily solved to yield

$$\sigma_0 = 0.96365173513.... \quad . \qquad (3.6.\ 7)$$

The expression (3.6. 6) also leads to an expansion for the boundary value $\varphi^\circ \equiv \varphi(x_0)$ of the form

$$\varphi^\circ = 144 \, x_0^{-3} \sum_{i=0}^{\infty} \overline{\pi}_i \, u_0^{\,i} \quad . \qquad (3.6.\ 8)$$

Values for σ_i and $\overline{\pi}_i$ are found in table 3.10. The complete discussion giving details of the methods adopted is contained in chapter 7.

In the next part of this thesis we will investigate in depth each of the topics only touched upon in the above highly condensed survey; this examination is the subject matter of chapters 4 to 7.

CHAPTER 4 . THE BAKER SERIES: ANALYSIS OF SERIES EXPANSIONS

We discuss the series solution to the TF equation due to Baker [1], defined by the boundary condition $\varphi(0) = 1$ and convergent near the origin. In the first section we show that it can be written formally as a double power series in $x^{\frac{1}{2}}$ and the initial slope B. The second section deals with general methods of infering the singular behaviour of a function from its power series. In the third and fourth sections this is applied to the Baker series in order to write it in the form of an expansion in powers of B for a fixed value of x, while in the last two sections we treat the expansion of φ in powers of $x^{\frac{1}{2}}$ for a fixed value of B.

4.1 . Formal solution to the TF equation near the origin

Our problem consists in solving the TF equation

$$\frac{d^2\varphi}{dx^2} = x^{-\frac{1}{2}}\,\varphi^{\frac{3}{2}} \quad , \tag{4.1. 1}$$

for small values of x with the boundary condition

$$\varphi(0) = 1 \quad . \tag{4.1. 2}$$

A general solution to the second-order equation (4.1. 1) contains two arbitrary parameters; since by the boundary condition one of these is fixed, we obtain a one-parameter family of solutions. The most convenient choice for this parameter is the slope of φ at the origin,

$$\varphi'(0) \equiv B \quad . \tag{4.1. 3}$$

As long as x is reasonably small, the Baker [1] solution (and therefore any transformations of it) is equally applicable to

- the isolated atom, for which $B = B_0$,
- the compressed atom [2], for which $B > B_0$, and
- the positive ion [3], for which $B < B_0$.

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1) E.B. Baker, Phys.Rev. 36 (1930) 630-47.

2) J.C. Slater & H.M. Krutter, Phys.Rev. 47 (1935) 559-68.

3) E. Guth & R. Peierls, Phys.Rev. 37 (1931) 217. The definition of positive ions given by Baker (ref.1) is false; this does not however affect his other results.

By a method of successive approximations, Baker [1] obtained the solution

$$\varphi(x) = 1 + \mathcal{B}x + \tfrac{4}{3}x^{\frac{3}{2}} + \tfrac{2}{5}\mathcal{B}x^{\frac{5}{2}} + \tfrac{1}{3}x^{3} + \tfrac{3}{70}\mathcal{B}^{2}x^{\frac{7}{2}} + \tfrac{2}{15}\mathcal{B}x^{4} + \left[\tfrac{2}{27} - \tfrac{1}{252}\mathcal{B}^{3}\right]x^{\frac{9}{2}} + \dots \quad . \tag{4.1.4}$$

By careful inspection of this expansion, we see that it can be written formally as

$$\varphi(x,\mathcal{B}) = \sum_{\ell=0}^{\infty}\sum_{s=0}^{\infty} a_{\ell,s}\, x^{\frac{3}{2}\ell+s}\,\mathcal{B}^{s} \quad , \tag{4.1.5}$$

indicating the dependence on $\mathcal{B}$ explicitly. The coefficients $a_{\ell,s}$ can be shown, by substitution in (4.1.1), to satisfy the simple recurrence relation

$$(3\ell+2s)(3\ell+2s-2)\,a_{\ell,s} = 4\,\tilde{a}_{\ell-1,s} \tag{4.1.6}$$

Here we have defined [+] the coefficients of the expansion of $\varphi^{\frac{3}{2}}$ as

$$\varphi^{\frac{3}{2}}(x,\mathcal{B}) = \sum_{\ell=0}^{\infty}\sum_{s=0}^{\infty} \tilde{a}_{\ell,s}\, x^{\frac{3}{2}\ell+s}\,\mathcal{B}^{s} \quad . \tag{4.1.7}$$

From (4.1.2/3) it follows immediately that

$$a_{0,0} = a_{0,1} = 1 \tag{4.1.8}$$

In table 4.1 the coefficients $a_{\ell,s}$ are listed for $0 \le \ell \le 8$, $0 \le s \le 8$.

In the following sections of this chapter we will analyse the expansion (4.1.5)

(a) by examining the functions of x multiplying each power $\mathcal{B}^{s}$, in order to establish an expansion of the type $\varphi(x\text{-const.},\mathcal{B})$, and

(b) by inspecting functions of x of the form $\varphi(x,\mathcal{B}=\text{const.})$.

First, however, some general methods will be outlined for obtaining

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[+] In this thesis we adopt the convention that, if $f(z) = \sum_{k=0}^{\infty} f_k z^k$ the coefficients of the expansion of $f^{\frac{3}{2}}(z)$ will be denoted by $\tilde{f}_k$: $f^{\frac{3}{2}}(z) = \sum_{k=0}^{\infty} \tilde{f}_k z^k$.

Table 4.1

The coefficients $a_{\ell,s}$ of the Baker series (4.1.5)

ℓ \ s	0	1	2	s / ℓ
0	.1000000000E+01	.1000000000E+01	.0000000000E-99	0
1	.1333333333E+01	.4000000000E-00	.4285714286E-01	1
2	.3333333333E-00	.1333333333E-00	.5714285714E-02	2
3	.7407407407E-01	.2087542088E-01	.5564435564E-02	3
4	.9876543210E-02	.5772005772E-02	-.1021201021E-02	4
5	.1918328585E-02	-.9591715474E-04	.1144651416E-02	5
6	.4853856706E-04	.4967774902E-03	-.7291196258E-03	6
7	.9508047845E-04	-.2394538197E-03	.5663380331E-03	7
8	-.3561524029E-04	.1685297738E-03	-.4467075818E-03	8

ℓ \ s	3	4	5	s / ℓ
0	.0000000000E-99	.0000000000E-99	.0000000000E-99	0
1	-.3968253968E-02	.9469696970E-03	-.3277972028E-03	1
2	.2539682540E-02	-.1195629767E-02	.6469720755E-03	2
3	-.1774928775E-02	.1315647976E-02	-.9646845949E-03	3
4	.1548081548E-02	-.1407495503E-02	.1292810326E-02	4
5	-.1284053635E-02	.1485383553E-02	-.1638274680E-02	5
6	.1136264426E-02	-.1560041961E-02	.2007203629E-02	6
7	-.1023576197E-02	.1636733233E-02	-.2404912916E-02	7
8	.9422516636E-03	-.1717414486E-02	.2836311887E-02	8

ℓ \ s	6	7	8	s / ℓ
0	.0000000000E-99	.0000000000E-99	.0000000000E-99	0
1	.1402243590E-03	-.6893382353E-04	.3741473974E-04	1
2	-.3848003848E-03	.2451578922E-03	-.1645938263E-03	2
3	.7306416745E-03	-.5688805627E-03	.4531415848E-03	3
4	-.1184781417E-02	.1086690445E-02	-.9989154334E-03	4
5	.1758682016E-02	-.1853347375E-02	.1927641551E-02	5
6	-.2467118283E-02	.2933380044E-02	-.3401458225E-02	6
7	.3327689180E-02	-.4402686755E-02	.5626559632E-02	7
8	-.4360741840E-02	.6350289317E-02	-.8862135188E-02	8

information about the location of, and the behaviour at, a singularity of a function by scrutinizing its power series expansion.

4.2 . **Function analysis from power series expansions**

In the course of this work we will very often want to gain insight in how a function behaves near a singularity and where the singularity is located. Our main item of information normally is the knowledge of a (limited) number of coefficients of the series expansion of the function. In the present section we will consider in detail how to solve this problem,with the Baker series as an illustration.

For convenience, define a function

$$\varphi_0(z) \equiv \sum_{l=0}^{\infty} a_{l,0}\, z^l \quad , \tag{4.2. 1}$$

where the coefficients are those of (4.1. 5). This function will serve to illustrate the methods to be developed.

The basis of our method is a theorem by Darboux [4], stating that late coefficients in a power series expansion are almost entirely determined by the behaviour of the function concerned near its singularities, in particular those nearest to the origin. To be specific, if a function $f(z)$ has a singularity (pole or branch point) of exponent α at z_0 and behaves for $z \approx z_0$ as

$$f(z) \approx \sum_{i=0}^{\infty} A_i \left(1 - \frac{z}{z_0}\right)^{-\alpha+i} \quad , \tag{4.2. 2}$$

then the coefficient f_k in

$$f(z) = \sum_{k=0}^{\infty} f_k\, z^k \tag{4.2. 3}$$

is given asymptotically as $k \to \infty$ by

$$f_k \approx \sum_{i=0}^{\infty} A_i\, z_0^{-k}\, \frac{(k+\alpha-i-1)!}{k!\,(\alpha-i-1)!} \quad . \tag{4.2. 4}$$

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4) G. Darboux, J.de Math. (3), 4 (1878) 5-56 and 376-85. For a short account, see e.g. G. Szegö, Orthogonal Polynomials, 2nd Ed., Am.Math.Soc., New York (1959) 204-6.

Table 4.2

The coefficients $a_{\ell,0}$ and their modified version according to (4.3.14) and (4.4.17)

ℓ	$a_{\ell,0}$	modified
0	.100000000000000E+01	.10812721315956 5E+01
1	.133333333333333E+01	.17133529432626 8E+01
2	.333333333333333E-00	.10466351646041 2E+01
3	.740740740740741E-01	.75814421256901 7E-00
4	.987654320987654E-02	.36073646793811 5E-00
5	.191832858499525E-02	.90 7646841964700E-01
6	.485385670570856E-04	.68147117136597 8E-02
7	.950804784463004E-04	-.41000 7462924821E-03
8	-.356152402936029E-04	.79145172341856 2E-04
9	.229943955776026E-04	-.19976930 3284811E-04
10	-.143896057914300E-04	.690837692720788E-05
11	.970316496053855E-05	-.27515781580435 1E-05
12	-.682830326566695E-05	.12482783039092 1E-05
13	.499191557514195E-05	-.62130 1094042647E-06
14	-.376623721938372E-05	.33358372893979 4E-06
15	.291889251680065E-05	-.19047938424907 8E-06
16	-.231511943473869E-05	.11450 8387413128E-06
17	.187356930841315E-05	-.71906679394970 7E-07
18	-.154326934665028E-05	.46879305715581 6E-07
19	.129124250353197E-05	-.31574917161888 9E-07
20	-.109554530245567E-05	.21883646799197 9E-07
21	.941208317921976E-06	-.15555517452760 0E-07
22	-.817790775491394E-06	.11309495745343 6E-07
23	.717864347541072E-06	-.83905213894046 2E-08
24	-.636048452762063E-06	.63396246825591 0E-08
25	.568382000679359E-06	-.48700093674796 9E-08

The ratio of the i-th to the $(i-1)$-th term in the sum (4.2. 4) is equal to $(\alpha - i)\, A_i \,/\, \{(k+\alpha-i)\, A_{i-1}\}$, showing that for very large k the first term in the sum will dominate. In that case, the coefficients f_k behave roughly like the expansion of the single power $A_0 (1 - z/z_0)^{-\alpha}$:

$$f_k \approx A_0 \, z_0^{-k} \, \frac{(k+\alpha-1)!}{k!\,(\alpha-1)!} \quad , \; k \to \infty \; . \tag{4.2. 5}$$

The expression (4.2. 5) behaves very regularly for large k ; the ratio

$$\frac{f_k}{f_{k-1}} = \frac{k+\alpha-1}{k} \; \frac{1}{z_0} \tag{4.2. 6}$$

approaches the constant value z_0^{-1} as $k \to \infty$.

We expect that the inverse of the statement above also holds: if the expansion of a function exhibits regular behaviour in its late coefficients, and if their ratios approach a constant value, then the function will have a singularity of the type described by (4.2. 2).

Let us first try to determine the location of the singularity (z_0) and the exponent there (α). As an example, consider the function $\varphi_0(z)$ defined by (4.2. 1), whose coefficients $a_{l,0}$ are given in the second column of table 4.2 . Let us define the ratio of successive coefficients

$$r_l = \frac{a_{l,0}}{a_{l-1,0}} \; . \tag{4.2. 7}$$

In the range of l -values for which (4.2. 5) holds, we expect r_l to be of the form (4.2. 6). Then z_0 and α can be found from two successive ratios by the relations

$$z_0^{-1} = l\, r_l - (l-1)\, r_{l-1} \quad ; \quad \alpha = z_0 \{ -l(l-2) r_l + (l-1)^2 r_{l-1} \} \; . \tag{4.2. 8}$$

For $21 \leq l \leq 25$, z_0^{-1} and α have been calculated from the above expressions; in table 4.3 we list the values obtained. These clearly

tend to a limit: extrapolating [5] to $\ell = \infty$, we find

$$z_0^{-1} \longrightarrow -1.0822 \quad ; \quad \alpha \longrightarrow -3.4996 \quad . \qquad (4.2.9)$$

Table 4.3 . Values of r_ℓ , z_0^{-1} and α .

ℓ	$-r_\ell$	$-z_0^{-1}$	$-\alpha$
21	0.8591231379	1.07273 149	3.18163 853
22	0.8688732982	1.07362 667	3.19566 151
23	0.8778092992	1.07440 132	3.20849 865
24	0.8860287531	1.07507 619	3.22029 488
25	0.8936143122	1.07566 773	3.23117 228

A second line of attack is aimed at finding values for the coefficients A_i in (4.2. 2), once reasonably accurate values for z_0 and α have been found. The result (4.2. 9) suggests that α is exactly equal to -3.5. Let us assume that this is so - it will be verified in the next section.

In order to calculate A_i , it is necessary to truncate the sum (4.2. 4), at $i = n$ say. Then we can find $A_0 \ldots A_n$ from $a_{\ell-n,0} \ldots a_{\ell,0}$ as follows:

$$\text{let } B_j = z_0^{\ell-j}\, a_{\ell-j,0}\, \frac{(\ell-j)!}{(\ell-n)!} \qquad \text{for } 0 \le j \le n \ , \qquad (4.2.10)$$

and define

$$\Delta_0^m = m! \sum_{j=m}^{n} (-)^j B_j \binom{n-m}{j-m} \frac{(\ell+\alpha-n-m-1)!}{(\ell+\alpha-n-j-1)!} \qquad \text{for } 0 \le m \le n \ . \qquad (4.2.11)$$

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5) H.E. Salzer, J.Math.and Phys. 33 (1954) 356-9.

Then if $\Delta_i^{m} = \Delta_{i-1}^{m} + \Delta_{i-1}^{m+1}$ for $1 \le i \le n$, $0 \le m \le n-i$, (4.2.12)

the coefficients A_i are given by

$$A_i = (-)^i \Delta_i^0 \binom{n}{i} \frac{(\ell-n)!\,(\alpha-i-1)!}{n!\,(\ell-n+\alpha-i-1)!} \quad . \tag{4.2.13}$$

By increasing n, or ℓ, or both, we obtain increasingly good estimates. For φ_0 one finds in this way:

$$A_0 \to -.0346 \; ; \; A_1 \to -.0264 \; ; \; A_2 \to -.019 \quad . \tag{4.2.14}$$

4.3 . <u>The Baker solution of intial slope zero</u>

The function $\varphi_0(z)$ introduced in the previous section is closely related to the general solution (4.1. 5); in fact for $B = 0$ this reduces to

$$\varphi(x, B=0) = \sum_{\ell=0}^{\infty} a_{\ell,0}\, x^{\frac{3}{2}\ell} = \varphi_0\left(x^{\frac{3}{2}}\right) . \tag{4.3. 1}$$

We have found that the late terms in the expansion of $\varphi_0(z)$ behave like those of

$$-.0346 \left(1 - \frac{z}{z_0}\right)^{\frac{7}{2}} + \ldots . \quad ; z_0 \simeq -.9240 \quad . \tag{4.3. 2}$$

Before going on to examine the coefficients $a_{\ell,s}$ for general values of s, let us examine the nature and the origin of the singularity in φ_0 more closely by means of the differential equation satisfied by it.

First of all, note that the singularity at z_0 is a "non-physical" one in the sense that in physical applications $z = x^{\frac{3}{2}}$ is always positive and therefore the singularity lies in a part of the complex z-plane that is not physically accessible. We will encounter this situation several times, in different contexts, in the course of this work; indeed, it is commonly found in many fields of physics. Van Dyke [6], in his book on fluid mechanics, gives a number of examples in that field where exactly the same situation

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6) M. Van Dyke, Perturbation Methods in Fluid Mechanics, Academic Press, New York/London (1964) 207-10.

occurs. (This book, displaying a wealth of mathematical techniques for dealing with mostly non-linear problems, is actually of very great interest to any physicist.)

In principle it must be possible to evade this difficulty, since a process of analytic continuation [7] can yield the function anywhere in the positive z-plane out to the nearest singularity, if any, in that half-plane. To see how this theoretical possibility can be carried through in practice we will now carefully inspect the function φ_0, since it is difficult to give hard-and-fast general rules on how to proceed in this type of situation.

Substitution of (4.3. 1) into the TF equation yields for φ_0 the equation:

$$9\, z\, \varphi_0''(z) + 3\, \varphi_0'(z) = 4\, \varphi_0^{\frac{3}{2}}(z) \quad . \tag{4.3. 3}$$

with the initial condition $\varphi_0(0) = 1$. It is easy to see that φ_0 is a monotonic increasing function of z; hence φ_0 intersects the z-axis at a non-vanishing angle for some negative value z_0 of z. Thus, for $z \approx z_0$, one finds that $\varphi_0 \propto (z - z_0)$. Obviously this leads immediately to a singular behaviour: near z_0 the right hand side of (4.3. 3) behaves like $(z - z_0)^{\frac{3}{2}}$ and after integration φ_0 contains a contribution behaving like $(z - z_0)^{\frac{7}{2}}$. The value of z_0 is determined as the smallest negative root of

$$\sum_{l=0}^{\infty} a_{l,0}\, z^l = 0 \quad ; \tag{4.3. 4}$$

anticipating the results of the remainder of this section, it is calculated very accurately as

$$z_0 = -.92398\ 64997\ 8649; \quad -z_0^{-1} = 1.0822\ 66894\ 8422 \quad . \tag{4.3. 5}$$

This confirms the results of the previous section, obtained directly from the numerical behaviour of the coefficients. We now see that $\alpha = -3.5$ exactly, while z_0 of (4.3. 5) replaces the estimate $-.9240$ of (4.2. 9).

To find an expansion of the form (4.2. 2) in powers of $\left(1 - \frac{z}{z_0}\right)$, we introduce into (4.3. 3) the new independent variable

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7) E.T. Wittaker & G.N. Watson, A Course of Modern Analysis, Camb.Univ.Press, 4th Ed. (1963) p. 140-2.

$$y = 1 - \frac{z}{z_0} \quad ; \quad z = z_0 (1-y) \; , \tag{4.3. 6}$$

in terms of which one obtains

$$9 (1-y) \varphi_0''(y) - 3 \varphi_0'(y) = 4 z_0 \varphi_0^{\frac{3}{2}}(y) \; . \tag{4.3. 7}$$

Furthermore, by the definition of z_0, $\varphi_0(y=0) = 0$. Around $y=0$ we write $\varphi(y) = E_0 y$, where

$$E_0 = - \sum_{l=0}^{\infty} l a_{l,0} \; z_0^{\,l} \; . \tag{4.3. 8}$$

Carrying out the summation with the value (4.3. 5) of z_0 one finds

$$E_0 = .81649\ 69574\ 9962 \; . \tag{4.3. 9}$$

If now we expand φ_0 in the form

$$\varphi_0(y) = \sum_{k=0}^{\infty} a_{k,0} \; y^{\frac{1}{2}k} \tag{4.3.10}$$

with $a_{0,0} = 0$ and $a_{2,0} = E_0$, then the coefficients $a_{7,0}$, $a_{9,0}$, ... will correspond to $A_0, A_1, \ldots$ of (4.2. 2). Letting $\tilde{a}_{k,0}$ represent the expansion coefficients of $\varphi_0^{\frac{3}{2}}(y)$ one is led from (4.3. 7) to the recurrence relation

$$9 k (k-2) a_{k,0} = (3k-6)(3k-10) a_{k-2,0} + 16 z_0 \tilde{a}_{k-4,0} \; . \tag{4.3.11}$$

In this way $\varphi_0(y)$ is found to be

$$\varphi_0(y) = E_0 y + \frac{1}{6} E_0 y^2 + \frac{2}{27} E_0 y^3 + \frac{16 z_0 E_0^{\frac{3}{2}}}{315} y^{\frac{7}{2}} + \frac{7}{162} E_0 y^4 + \frac{332 z_0 E_0^{\frac{3}{2}}}{8505} y^{\frac{9}{2}} + \frac{7}{243} E_0 y^5 + \frac{611 z_0 E_0^{\frac{3}{2}}}{20790} y^{\frac{11}{2}} + \ldots \; . \tag{4.3.12}$$

Finally, substitution of numerical values for z_0 and E_0 yields

$$a_{7,0} = A_0 = -.03462\ 63656\ldots \; ; \; a_{9,0} = A_1 = -.02661\ 10032\ldots \; ; \; a_{11,0} = A_2 = -.02003\ 47627\ldots \tag{4.3.13}$$

replacing our earlier estimates (4.2.14) which were the results of direct examination of the coefficients $a_{l,0}$.

In (4.3.12) the terms containing y, y^2, y^3 are dominant and give major contributions to the coefficients $a_{l,0}$ for lower l-values; therefore it is impossible to obtain more strongly convergent expansions by a simple transformation of variables, as for instance an Euler transformation [6]. One can, however, write φ_0 in a form separating the first few singular terms:

$$\varphi_0(z) = d_{7,0}\left(1-\frac{z}{z_0}\right)^{\frac{7}{2}} + d_{9,0}\left(1-\frac{z}{z_0}\right)^{\frac{9}{2}} + \ldots$$
$$+ \sum_{l=0}^{\infty} z^l \left[a_{l,0} - \frac{1}{z_0^l\, l!}\left\{ \frac{(l-\frac{9}{2})!}{(-\frac{9}{2})!}\, d_{7,0} + \frac{(l-\frac{11}{2})!}{(-\frac{11}{2})!}\, d_{9,0} + \ldots \right\} \right] . \qquad (4.3.14)$$

By separating out more and more terms of the type $\left(1-\frac{z}{z_0}\right)^{\frac{7}{2}+b}$, $b = 0,1,2\ldots$ the remaining coefficients in the square brackets can be made smaller and smaller, especially for large values of l. When three contributions are subtracted in this way, the resulting coefficients are as listed in table 4.2 on page 46, the 3rd column. The coefficients of the new series are about a factor 10^2 smaller than the original $a_{l,0}$. In fact (4.3.14) was employed to find the accurate values (4.3. 4) and (4.3. 9) in an iterative manner. We also applied the convergence-accelerating techniques described in appendix 10.2.

4.4 . The full Baker solution as a perturbation expansion

Let us now return to our original aim: to write $\varphi(x,\mathcal{B})$ as an explicit function of $\mathcal{B}$ for given x. Analogous to (4.2. 1) we define functions

$$\varphi_s(z) \equiv \sum_{l=0}^{\infty} a_{l,s}\, z^l \quad , \qquad (4.4.\ 1)$$

in terms of which the Baker solution (4.1. 5) may be written as

$$\varphi(x,\mathcal{B}) = \sum_{s=0}^{\infty} \varphi_s\left(x^{\frac{3}{2}}\right) (x\mathcal{B})^s \quad . \qquad (4.4.\ 2)$$

For a fixed value of $\varkappa$, define

$$\ell_s(\varkappa) = \varkappa^s \varphi_s(\varkappa^{\frac{3}{2}}) \qquad (4.4.\ 3)$$

so that

$$\varphi(\varkappa = const., \mathcal{B}) = \sum_{s=0}^{\infty} \ell_s \mathcal{B}^s \quad . \qquad (4.4.\ 4)$$

Similarly define

$$\ell_s'(\varkappa) = \varkappa^s \left[s\varphi_s(\varkappa^{\frac{3}{2}}) + \tfrac{3}{2} \varkappa^{\frac{3}{2}} \varphi_s'(\varkappa^{\frac{3}{2}}) \right], \qquad (4.4.\ 5)$$

from which

$$\varkappa \varphi'(\varkappa = const., \mathcal{B}) = \sum_{s=0}^{\infty} \ell_s' \mathcal{B}^s \quad . \qquad (4.4.\ 6)$$

Our problem will now be solved if we can accurately perform the summations implicit in (4.4. 3/5) for $\varkappa$ as large as 1. To this end the expansions (4.4. 1) are scrutinized in much the same way as before.

Applying the methods of section 4.2 to the expansion coefficients $a_{\ell,s}$ for a given s we easily establish the following facts empirically:

(i) φ_s contains contributions of the form

$$\sum_{i=0}^{\infty} A_i^{(s)} \left(1 - \frac{z}{z_0}\right)^{-\alpha_s + i} \quad , \qquad (4.4.\ 7)$$

where $z_0 \approx -.924$ (as for φ_0) and $\alpha_s = -3.5 + s$; (4.4. 8)

(ii) the coefficients $A_0^{(s)}$ in turn form a regular sequence which can be fitted to an expression of the form

$$A_0^{(s)} \approx -.0346 \binom{\frac{7}{2}}{s} 0.9^s \quad . \qquad (4.4.\ 9)$$

To explain these remarkable regularities, we substitute (4.4. 2) into the TF equation in order to obtain a differential equation for $\varphi_s(z)$:

$$9 z^2 \varphi_s''(z) + 3(4s+1) z \varphi_s'(z) + 4s(s-1) \varphi_s(z) = 4z \tilde{\varphi}_s(z). \qquad (4.4.10)$$

Here $\tilde{\varphi}_s$ is defined in a manner analogous to (4.1. 6) and (4.4. 1/2):

$$\tilde{\varphi}_s(z) = \sum_{l=0}^{\infty} \tilde{a}_{l,s}\, z^l \quad ; \quad \varphi^{\frac{3}{2}}(x,\mathcal{B}) = \sum_{s=0}^{\infty} \tilde{\varphi}_s(x^{\frac{3}{2}})\,(x\mathcal{B})^s . \qquad (4.4.11)$$

For $s=0$, equation (4.4.10) reduces to (4.3. 3) for φ_0 ; for $s>0$ it is an inhomogeneous, but linear equation. The "source" term contains contributions like

$$\varphi_0^{\frac{3}{2}-s}\,\varphi_1^{\,s} \quad , \quad \varphi_0^{\frac{5}{2}-s}\,\varphi_1^{\,s-2}\,\varphi_2 \quad , \qquad \text{etc.} \; . \qquad (4.4.12)$$

These forms are easily derived with the help of a simple algorithm described in appendix 10.33.

As in the previous section, we introduce the independent variable $y = 1 - z/z_0$ and write

$$\varphi_s(y) = \sum_{k=0}^{\infty} a_{k,s}\, y^{\frac{1}{2}k} \qquad (4.4.13)$$

From (4.4.12) it is obvious that the lowest term in (4.4.13) with an odd k -value is given by $k = 7-2s$, giving rise to terms of the form $(1 - z/z_0)^{\frac{7}{2}-s}$ etc., in accordance with (4.4.8). The coefficients $a_{7-2s,s}$, $a_{9-2s,s}$, ... which are the same as $A_0^{(s)}$, $A_1^{(s)}$, ... in (4.4. 7) can easily be calculated explicitly. For the first few of these we find, defining (see table 4.4)

$$\mathcal{D}_s = \varphi_s \Big|_{z=z_0} \quad , s = 0,1,2,3 \quad ; \quad E_s = -z_0 \left.\frac{d\varphi_s}{dz}\right|_{z=z_0} \quad , s = 0,1,2 \quad ; \qquad (4.4.14)$$

Table 4.4 . Numerical values of $\mathcal{D}_s$ and E_s.

s	$\mathcal{D}_s$	E_s
0	.00000 00000	.81649 69575
1	.73281 28953	.16736 70181
2	-.04288 77610	.09010 11748
3	.02061 74675	———

$$d_{7-2s,s} = \frac{16 z_0}{315} \binom{\frac{7}{2}}{s} E_0^{\frac{3}{2}-s} D_1^{s} \;;$$

$$d_{9-2s,s} = \frac{4 z_0}{8505} \binom{\frac{9}{2}}{s} E_0^{\frac{3}{2}-s} D_1^{s-2}$$

$$\times \left[(83 - 85 + 45^2) D_1^2 + 12 \binom{s}{1} (5-2s) D_1 E_1 + 48 \binom{s}{2} E_0 D_2 \right] \;;$$

$$d_{11-2s,s} = \frac{z_0}{1683990} \binom{\frac{11}{2}}{s} E_0^{\frac{3}{2}-s} D_1^{s-4}$$

$$\times \Big[(49491 - 4496\, s + 3240 s^2 - 448 s^3 + 48 s^4) D_1^4$$
$$+ 72 \binom{s}{1} (5-2s)(183 - 32 s + 4 s^2) D_1^3 E_1$$
$$+ 288 \binom{s}{2} \{ (127 - 16 s + 4 s^2) E_0 D_1^2 D_2 + 3(5-2s)(7-2s) D_1^2 E_1^2$$
$$+ 12 (7-2s) E_0 D_1^2 E_2 \}$$
$$+ 10\,378 \binom{s}{3} \{ (7-2s) E_0 D_1 E_1 D_2 + 2 E_0^2 D_1 D_3 \}$$
$$+ 41472 \binom{s}{4} E_0^2 D_2^2 \Big] \;. \qquad (4.4.15)$$

In principle we could carry on in this way, but the complicated nature of the coefficients soon renders this procedure impracticable. When we substitute numerical values as listed in table 4.4 , the first expression in (4.4.15) reduces to

$$d_{7-2s,s} = A_0^{(s)} = -.03462\;63657 \binom{\frac{7}{2}}{s} .89750\;81763^{s} \;, \qquad (4.4.16)$$

replacing the earlier, empirical estimate (4.4. 9).

We can now follow two methods to sum $\varphi_s(x^{\frac{1}{2}})$ accurately for $x=1$, say:

(i) for s = 0, 1, 2, 3, 4 apply the method of (4.3.14), i.e. write

$$\varphi_s(z) = \sum_{i=0}^{n} d_{7-2s+2i,s} \left(1 - \frac{z}{z_0}\right)^{\frac{7}{2}-s+i}$$
$$+ \sum_{l=0}^{\infty} z^l \left[a_{l,s} - \frac{1}{z_0^l\, l!} \sum_{i=0}^{n} d_{7-2s+2i,s} \frac{(l+s-i-\frac{9}{2})!}{(3-i-\frac{1}{2})!} \right] \;, \qquad (4.4.17)$$

Table 4.5

The coefficients $a_{\ell,10}$ and their modification $a^{*}_{\ell,10}$ according to (4.4.19)

ℓ	$a_{\ell,10}$	$a^{*}_{\ell,10}$
0	.000000000000000E-99	.000000000000000E-99
1	.135528374902950E-04	.135528374902950E-04
2	-.833264571007512E-04	.120141606542419E-04
3	.303496532904190E-03	.107298841168667E-05
4	-.851366184424532E-03	-.306416565279315E-06
5	.203088945356593E-02	.973473956350586E-07
6	-.433135001742279E-02	-.429649788525769E-07
7	.850515103722642E-02	.190408989946264E-07
8	-.156695187563799E-01	-.942356314157212E-08
9	.274379283283314E-01	.508909247005201E-08
10	-.460882509006966E-01	-.293593994111300E-08
11	.747760265800976E-01	.178738323259592E-08
12	-.117802923753957E-00	-.113761031921458E-08
13	.180952391950999E-00	.751722124451799E-09
14	-.271906799716732E-00	-.512984300934741E-09
15	.400763024596246E-00	.360011453175922E-09
16	-.580666590969724E-00	-.258957695261512E-09
17	.828588103994945E-00	.190387619154698E-09
18	-.116626998546899E+01	-.142739304759690E-09
19	.162137647303730E+01	.108917487105507E-09
20	-.222888560430900E+01	-.844460651978728E-10
21	.303276859383673E+01	.664305752239864E-10
22	-.408800976272809E+01	-.529571371826630E-10
23	.546302915677175E+01	.427344225755961E-10
24	-.724258037070903E+01	-.348749554553739E-10
25	.953120809044091E+01	.287584400829857E-10

taking as many terms in the first sum as one can - and wants to - calculate. For low values of s a small value of m is sufficient to make the expressions in square brackets in (4.4.17) much smaller than the original coefficients $a_{\ell,s}$ (for an example see table 4.2 , on page 46. For higher values $s>4$ however, a very high value of m would have to be adopted in order to obtain any improvement over the original expansion (4.4. 1). Thus, we turn to a different method:

(ii) for $s \geq 5$ we write φ_s in the form

$$\varphi_s(z) = \left(1 - \frac{z}{z_0}\right)^{\frac{7}{2}-s} \varphi_s^*(z) \quad . \qquad (4.4.18)$$

Here

$$\varphi_s^*(z) = \sum_{\ell=0}^{\infty} a_{\ell,s}^* z^\ell \qquad \text{with} \quad a_{\ell,s}^* = \sum_{m=0}^{\ell} z_0^m \binom{m-s+\frac{7}{2}}{m} a_{\ell-m,s} \quad . (4.4.19)$$

The factor $\left(1 - \frac{z}{z_0}\right)^{\frac{7}{2}-s}$ completely dominates the form of the coefficients $a_{\ell,s}$ in this range of s , and hence (4.4.19) shows a tremendous improvement. As an example we have listed numerical values of $a^*_{\ell,10}$ together with $a_{\ell,10}$ in table 4.5 . We note that $a^*_{20,10}$ is smaller than $a_{20,10}$ by a factor 10^{11} !

These types of method, and the application of special summation techniques as described in appendix 10.2 , yield accurate values for b_s and b_s' . These coefficients are listed in table 3.1 , taking $\varkappa = 1$ in (4.4. 3/5). In the calculation of $a^*_{\ell,s}$ by (4.4.19) large cancellation losses occur; therefore we calculated $a_{\ell,s}$ to 28 figures on the IBM 1620, rounding off the resultant coefficients $a^*_{\ell,s}$ to 16 figures before processing them further.

4.5 . The Baker solution for fixed initial slope B

Once in a particular situation the value of B has been determined, the procedures of the previous section are not particularly convenient. Instead an expression is needed for $\varphi(\varkappa, B = const.)$ with special emphasis on convenience of numerical evaluation. To this end, we first define coefficients

$$a_k(\mathcal{B}) = \sum_{3l+2s=k} a_{l,s}\, \mathcal{B}^s \quad . \qquad (4.5.\ 1)$$

in terms of which (4.1. 5) may be written as

$$\varphi(x,\ \mathcal{B} = const.) = \sum_{k=0}^{\infty} a_k\, x^{\frac{1}{2}k} \quad . \qquad (4.5.\ 2)$$

In practice, it is easier to calculate the a_k directly by means of the recursion relation

$$k(k-2)\ a_k = 4\ \tilde{a}_{k-3} \quad , \quad k \geq 3 \quad , \qquad (4.5.\ 3)$$

starting from the obvious values $a_0 = 1, a_1 = 0, a_2 = \mathcal{B}$ (cf. also equation (4.1. 4)). Here $\tilde{a}_k$ denote the expansion coefficients of $\varphi^{\frac{3}{2}}$ in powers of $x^{\frac{1}{2}}$. The values a_k obtained by means of (4.5. 3), with the isolated-atom value $\mathcal{B}_0 = -1.588071022 6$ for $\mathcal{B}$, are listed in table 3.2 on page 30. These values will be employed to illustrate the general properties of the function (4.5. 2) - properties whose nature is independent of the particular value of $\mathcal{B}$ chosen.

Let us define for the purpose of the analysis a function

$$f(z) \equiv \sum_{k=0}^{\infty} a_k\, z^k \quad ; \quad \varphi(x) = f(x^{\frac{1}{2}}) \quad . \qquad (4.5.\ 4)$$

This function is analysed in the same way as φ_0 in section 4.2 . From the expansion (4.5. 4) we deduce that it contains terms of the form

$$\left(1 - \frac{z}{z_0}\right)^{3.5+i} \quad ; \quad z_0 \approx -.66525 \quad . \qquad (4.5.\ 5)$$

By substituting (4.5. 4) into the TF equation one derives that $f(z)$ satisfies the differential equation

$$z\, f''(z) - f'(z) = 4 z^2 f^{\frac{3}{2}}(z) \quad . \qquad (4.5.\ 6)$$

Like φ_0 in the previous sections, the function $f(z)$ is monotonic increasing, at least for negative values of z . It intersects the z-axis at

$$z = z_0 = -.66523\ 94668\ \ldots \quad , \qquad (4.5.\ 7)$$

while in that point the derivative $f'(z)$ is non-zero, leading to

$$A \equiv -z_0 \left.\frac{df}{dz}\right|_{z=z_0} = -\sum_{k=0}^{\infty} k a_k z_0^k = 2.12305\ 95046\ldots \quad (4.5.8)$$

Defining, in analogy with (4.3.12), $y = 1 - z/z_0$, we obtain

$$f(y) = Ay - \tfrac{1}{2}Ay^2 + \tfrac{16}{35}z_0^3 A^{\frac{3}{2}} y^{\frac{7}{2}} - \tfrac{172}{315} z_0^5 A^{\frac{5}{2}} y^{\frac{9}{2}} + \tfrac{79}{462} z_0^3 A^{\frac{3}{2}} y^{\frac{11}{2}} + \ldots \quad (4.5.9)$$

However, the improvement in convergence obtained by subtracting the contributions (4.5.5) multiplied by appropriate coefficients taken from (4.5.9) is hardly worthwhile. We do nevertheless get an accurate value for the radius of convergence of $\varphi(x^{\frac{1}{2}})$; for from (4.5.7) it follows that

$$x_0 = z_0^2 = .44254\ 35482\ldots \quad (4.5.10)$$

This contrasts with the method employed by Enstrom [8] to determine x_0 ; he calculates 730 coefficients of (4.5.2), still obtaining only the very rough estimate $x_0 \approx .44$. In addition we want to remark that our recursion formula (4.5.3) is far simpler and certainly entails much less work than Enstrom's. The reason is that Enstrom has to square both sides of the TF equation in order to remove the $\frac{3}{2}$ power, thus arriving at a formula in which the number of operations increases quadratically with k ; while we employ a simple algorithm (appendix 10.33) to obtain $\tilde{a}_k$, which involves an only linearly increasing number of terms.

The conclusion that can be drawn from the above analysis of the series (4.5.2) is that this time elucidating the structure does not assist us greatly in procuring a faster converging replacement for it. To attain sufficient accuracy near $x = 1$, we replace the series by the equivalent Padé approximants, discussed in the following section.

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8) J.E. Enstrom, J.Chem.Phys. 46 (1967) 1213-4.

4.6 . Padé approximants to the Baker solution

Specially for use in numerical applications we express $\varphi(x)$ and $\varphi'(x)$ as rational approximations to their power series expansion (4.5. 2). As is well known [9], the Padé approximants are the "best" rational approximations of given order to a power series in the sense that the (n,m) approximant to the series $\sum_{k=0}^{\infty} a_k z^k$ is that ratio of two polynomials $P_m(z)$ and $Q_n(z)$, of degree $\leq m$ and $\leq n$ resp., whose power series expansion agrees with the original series up to at least the $(n+m)$th power of z :

$$(n,m) = \frac{P_m(z)}{Q_n(z)} \quad ; \quad \frac{P_m(z)}{Q_n(z)} - \sum_{k=0}^{\infty} a_k z^k = O(z^{m+n+1}) \qquad (4.6.\ 1)$$

The relation (4.6. 1) uniquely determines the coefficients p_i and q_i of the polynomials P_m and Q_n ; they can explicitly be written [9] as $(n+1)\times(n+1)$ determinants involving the coefficients a_k . Since this involves a huge amount of tedious calculation, prohibitively so for larger n , we have developed a simpler way to calculate p_i and q_i , making use of the known [10] connection between Padé approximants and continued-fraction representations of the function $f(z)$. (Our thanks are due to Mr. A.T. Davie for drawing our attention to this connection). The details are relegated to appendix 10.36.

To represent $\varphi(x)$ and $\varphi'(x)$ accurately in the interval $0 \leq x \leq 1$ we have chosen the (12,14) approximants

$$\varphi(x) = \frac{\sum_{i=0}^{14} p_i\, x^{\frac{1}{2}i}}{\sum_{i=0}^{12} q_i\, x^{\frac{1}{2}i}} \quad ; \quad \varphi'(x) = \frac{\sum_{i=0}^{14} p_i'\, x^{\frac{1}{2}i}}{\sum_{i=0}^{12} q_i'\, x^{\frac{1}{2}i}} \quad . \qquad (4.6.\ 2)$$

The numerical values of the coefficients are collected in table 3.3 on page 31. These expressions yield values of $\varphi(x)$ and $\varphi'(x)$ accurate to at least 12 significant figures for $x \leq 1$, and still to 9 figures even for $x \approx 2$.

This completes our description of the TF function for values of x near the origin. In the following two chapters we will discuss its behaviour for large x; this has to be done separately for isolated and for compressed atoms.

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9) for a survey, see G.A. Baker Jr, Adv.in Theor.Phys. 1 (1965) 1-58.

10) H.S. Wall, Analytic Theory of Continued Fractions, Van Nostrand New York - Toronto - London, (1948).

CHAPTER 5 . THE COULSON-MARCH SOLUTION FOR THE ISOLATED ATOM

When examining the TF function for large positive values of x, one must distinguish between the isolated atom for which x ranges to infinity, and the compressed atom for which it is limited to values less than the boundary radius x_0. This contrasts with the discussion of the previous chapter, where the same expansion was applicable to either of these cases. In this chapter the first case will be treated, that of the isolated atom. The more general problem of the compressed atom will be left until the next chapter.

5.1 . The formal asymptotic solution of Coulson and March

The essential aims of this chapter can be stated as

(i) to find a solution to $\frac{d^2\varphi}{dx^2} = x^{-\frac{1}{2}}\varphi^{\frac{3}{2}}$, $\varphi(\infty)=0$, (5.1. 1)
for values of $x \gg 1$, and

(ii) to extend this solution so that it can be made to yield accurate numerical values for φ even when $x \to 1$.

In this section we concentrate on (i); the extension to a wider range of x -values is the subject of the remaining sections.

Since in (5.1. 1) we impose only one boundary condition, we expect to obtain a one-parameter set of solutions. As Sommerfeld [1] has already shown, a particular solution to this equation is

$$\varphi(x) = 144\, x^{-3} \quad ; \qquad (5.1.\ 2)$$

he also proves that any solution to (5.1. 1) satisfying the boundary condition must ultimately behave like (5.1. 2). This leads us to write, following Coulson and March [2,3]

$$\varphi(x) = 144\, x^{-3}\, \psi(x) \quad ; \quad \lim_{x\to\infty} \psi(x) = 1 \, . \qquad (5.1.\ 3)$$

The additional condition that $\psi(\infty) = 1$, being a direct consequence of the fact that x ranges to ∞ and of the boundary condition

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1) A. Sommerfeld, Z.f.Phys. 78 (1932) 283-308.

2) C.A. Coulson & N.H. March, Proc.Phys.Soc.A 63 (1950) 367-74, referred to as CM.

3) N.H. March, Proc.Camb.Phil.Soc. 48 (1952) 665-82.

(5.1. 1), creates the essential difference alluded to above between this and the compressed-atom solution. Substitution in the TF equation yields

$$x^2 \frac{d^2\psi}{dx^2} - 6\, x \frac{d\psi}{dx} + 12\,\psi = 12\,\psi^{\frac{3}{2}} \quad . \qquad (5.1.\ 4)$$

Still following CM we attempt to write $\psi(x)$ as a power series in some - not necessarily integer - power x^λ :

$$\psi = 1 - F x^\lambda + \dots \quad . \qquad (5.1.\ 5)$$

On insertion of (5.1. 5) in the differential equation a necessary condition on F and λ turns out to be $F(\lambda^2 - 7\lambda - 6) = 0$, whence

$$\left.\begin{aligned} \lambda &= \lambda_+ = \tfrac{7+\sqrt{73}}{2} = 7.772001872658765\dots \\ \text{or} \quad \lambda &= \lambda_- = \tfrac{7-\sqrt{73}}{2} = -.772001872658765\dots \end{aligned}\right\} \qquad (5.1.\ 6)$$

while F remains arbitrary. Since $x^{\lambda_+} \to \infty$ as $x \to \infty$, in order to satisfy the condition $\psi(\infty) = 1$ one can retain here only the negative root λ_- .

We can now write (5.1. 5) formally as

$$\psi = \psi(z) = \sum_{k=0}^{\infty} e_k z^k \quad ; \quad z = F x^{\lambda_-} \quad , \qquad (5.1.\ 7)$$

where the e_k are numerical constants depending only on k and λ_- while the arbitrary constant F , the parameter distinguishing different solutions of this family, is included in the new independent variable z . With CM we choose $e_1 = -1$; this choice of sign ensures that for the isolated atom F is positive. Defining, for convenience,

$$\mu \equiv \frac{\lambda_-^2}{6} = .099331148564773\dots \qquad (5.1.\ 8)$$

we rewrite (5.1. 4) in the form

$$\mu z^2 \frac{d^2\psi}{dz^2} + z \frac{d\psi}{dz} + 2\psi = 2\psi^{\frac{3}{2}} \quad . \qquad (5.1.\ 9)$$

With the usual definition of $\tilde{e}_k$ as the expansion coefficient of $\psi^{\frac{3}{2}}$, one derives for e_k the relation

$$(k-1)(\mu k + 1)\, e_k = 2\left(\tilde{e}_k - \tfrac{3}{2} e_k\right) \quad . \qquad (5.1.10)$$

This recurrence relation enables us to calculate c_k quite easily, starting from $c_0 = 1$, $c_1 = -1$. The coefficients of the solution defined in this way, usually referred to as the Coulson-March asymptotic solution, are listed in table 3.4 on page 33.

5.2 . Analysis of the Coulson-March series

The decrease in magnitude of the coefficients c_k of (5.1. 7) is so slow that this expansion is inapplicable at values of $x \lesssim 10$. Since φ and thus ψ have to be evaluated for $x \approx 1$ we first examine the series to see what singularity limits its range of convergence.

By inspection the coefficients for $k \geq 2$ are seen to behave very regularly, having a nearly constant ratio; thus we are led to apply Darboux's theorem as in section 4.2 . Trying to fit c_k to a functional form

$$c\,(1+\beta z)^{-\alpha} \qquad (5.2.\ 1)$$

and after analysis entirely parallel to that of section 4.2 we find

$$\alpha \approx 3.997 \quad ; \quad \beta \approx .25077 \ , \qquad (5.2.\ 2)$$

suggesting that $\alpha = 4$ exactly. This conclusion also follows from two alternative approaches, as follows.

First, substitute the expected form (5.2. 1) into the recursion formula (5.1.10); with

$$c_k = c\,(-\beta)^k \ \frac{(k+\alpha-1)!}{k!\,(\alpha-1)!} \ , \quad \tilde{c}_k = e^{\frac{3}{2}}(-\beta)^k \ \frac{(k+\tfrac{3}{2}\alpha-1)!}{k!\,(\tfrac{3}{2}\alpha-1)!} \ , \qquad (5.2.\ 3)$$

and expanding the factorials on both sides for large k , we arrive at

$$\frac{\mu c}{(\alpha-1)!}\ k^{\alpha+1} \approx \frac{2\,e^{\frac{3}{2}}}{(\tfrac{3}{2}\alpha-1)!}\ k^{\frac{3}{2}\alpha-1} \ , \qquad (5.2.\ 4)$$

retaining only the leading terms in k. From this it follows that

$$\alpha = 4 \ , \ \beta = \text{arbitrary}, \ c \approx 0.98 \ . \qquad (5.2.\ 5)$$

Further examination shows that the approximation (5.2. 4), retaining only the leading terms in k , is justified for $k/0.067 \gg 1$, i.e. for all relevant k.

The other way to approach the problem is to note that to within less than 1%, the value (5.1. 8) of μ is equal to 0.1. Thus solving (5.1. 9) with μ replaced by 0.1 we expect a solution which is very close to the true solution. Denoting this approximate solution by $\psi_{0.1}$ this leads immediately to the equation

$$\tfrac{1}{10} z^2 \psi_{0.1}'' + z \psi_{0.1}' + 2\psi_{0.1} = 2\psi_{0.1}^{\frac{3}{2}} , \qquad (5.2.\ 6)$$

which has the exact solution

$$\psi_{0.1} = (1+\beta z)^{-4} . \qquad (5.2.\ 7)$$

The requirement that $\psi_{0.1} = -1$ then fixes $\beta = 0.25$.

Thus all three lines of attack provide convincing evidence that the main singularity of $\psi(z)$ as a function of z is a fourth-order pole. In itself, this is nothing new; Thomas [4] in his original paper implies a behaviour of this kind. In addition Brillouin [5] has pointed out that any solution whose initial slope is higher than that for the isolated atom must go to infinity as a 4th order pole at some finite x. However, he rejected the part of the solution beyond the pole as unphysical. In the next section we will see how this part, which corresponds to the CM solution for negative z, can be given a meaningful place in the TF theory.

5.3. The CM solution re-expressed in a manner suitable for all values of the parameter

Knowing that $\psi(z)$ behaves almost like $(1+\beta z)^{-4}$, we are tempted to write

$$\psi(z) = \left[\sum_{k=0}^{\infty} \delta_k z^k\right]^{-4} \qquad (5.3.\ 1)$$

expecting that the values of δ_k for $k \geq 2$ will be very small. In principle one could calculate the coefficients of (5.3. 1) as the expansion of $\psi^{-\frac{1}{4}}$ (see appendix 10.33), but severe cancellation

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4) L.H. Thomas, Proc.Camb.Phil.Soc. 23 (1927) 542-8.

5) L. Brillouin, L'atome de Thomas-Fermi, Actualités Scientifiques et Industrielles No. 160, Hermann, Paris (1934).

losses limit this procedure to only the first few coefficients. Instead, substituting (5.3. 1) directly into (5.1. 9) we obtain the recursion relation

$$2(k-1)(\mu k+1)\,\delta_k = \sum_{\ell=1}^{k-1} \left[5\mu k^2 + (\mu-1)k + 1 - 12\mu\ell^2 \right] \delta_\ell\, \delta_{k-\ell} \cdot (5.3.\ 2)$$

Starting from $\delta_0 = 1$, $\delta_1 = 0.25$ one finds the values δ_k as listed in table 3.5 on page 33. We observe a tremendous improvement in the magnitude of the coefficients, δ_{30} being smaller than c_{30} by a factor 10^{16}.

Let us determine the exact location of the pole of $\psi(z)$: it must be the nearest negative root of $\sum_{k=0}^{\infty} \delta_k z^k = 0$. For z_0 one obtains

$$z_0 = -3.9878\ 39025\ 608168\ ;\ \beta = -z_0^{-1} = .25076\ 23787\ 165016\ ;\ (5.3.\ 3)$$

this replaces our earlier estimate $\beta \approx .25077$ of (5.2. 2), obtained directly from the numerical behaviour of the coefficients c_k .

For large k the δ_k behave roughly like the coefficients of a hypergeometric series with radius of convergence $|z_0|$. Since the series as it stands yields quite accurate enough values for our purposes, and since in the next section we will develop a formulation which is still better for isolated-atom solutions, we have not pursued this matter further.

The singularity of $\psi(z)$ lies on the negative z-axis, as is shown by (5.3. 3). Whether or not in an actual case z takes on negative values is determined by the sign of the parameter F , as can be seen from (5.1. 7). All solutions to (5.1. 1) which lie below the Sommerfeld solution (5.1. 2) have positive values of F ; for these the singularity is never actually reached as x varies. Therefore it is possible to remove the singularity entirely: we have once again a "physically inaccessible" singularity. The treatment of this type of solution (the isolated atom belongs to this class) is given in the next section.

For those solutions lying above the Sommerfeld solution, F is negative; these curves actually do show the 4th order pole as x decreases from infinity (z decreases from 0). They are the large-x

parts of the curves found by Brillouin and mentioned in section 5.2. March [3] has shown that these solutions can be necessary to describe the TF field of molecules with tetrahedral or octahedral symmetry. He has to use numerical integration to find these functions; in appendix 10.12 we show how our form (5.3. 1) can easily yield numerical values for March's "Master Solutions", defined by the typical parameter values $F = \pm 1$.

5.4 . Re-expression of the CN solution valid only for positive parameter

In the previous section we observed already that for the solutions below the Sommerfeld solution (5.1. 2) the singularity lies in an inaccessible part of the complex z-plane. This is a situation similar to that encountered in section 4.3; in the present case an Euler-type transformation meets our needs exactly.

Let us define a new variable

$$u = \frac{\beta z}{1+\beta z} \quad , \quad \beta z = \frac{u}{1-u} \quad , \qquad (5.4.\ 1)$$

with β given by (5.3. 3). The singularity at z_0 is by this transformation moved to the point at infinity, and the resulting series in u should converge for $0 \leq u < 1$, corresponding to $\infty \geq z > 0$. The dominating $(1+\beta z)^{-4}$ dependence changes into $(1-u)^4$, which is entirely harmless. As in the previous section, calculation of the new expansion coefficients from c_k is effectively prevented by cancellation losses; therefore we derive a new recursion relation. In terms of u the differential equation for ψ is

$$\mu (1-u^2) u^2 \frac{d^2\psi}{du^2} + (1-u)(1-2\mu u) u \frac{d\psi}{du} + 2\psi = 2\psi^{\frac{3}{2}} . \qquad (5.4.\ 2)$$

and with the expansions

$$\psi(u) = \sum_{k=0}^{\infty} \gamma_k u^k \quad , \quad \psi^{\frac{3}{2}}(u) = \sum_{k=0}^{\infty} \tilde{\gamma}_k u^k , \qquad (5.4.\ 3)$$

we easily derive

$$(k-1)(\mu k+1)\,\gamma_k = (k-1)(1+2\mu(k-1))\,\gamma_{k-1} + \mu(k-1)(k-2)\gamma_{k-2} + 2(\tilde{\gamma}_k - \tfrac{3}{2}\gamma_k) \quad . \qquad (5.4.\ 4)$$

From (5.4. 1) and $c_1 = -1$ it follows that $\gamma_1 = -1/\beta = z_0$.
Since $x\,\frac{d}{dx} \rightarrow \lambda_-(1-u)u\,\frac{d}{du}$ we can write $\varphi'(x)$ as

$$\varphi'(x) = 144\,x^{-4}\sum_{k=0}^{\infty}\gamma'_k\,u^k \quad , \qquad (5.4.\ 5)$$

where

$$\gamma'_k = (-3+k\lambda_-)\gamma_k - (k-1)\lambda_-\gamma_{k-1} \quad . \qquad (5.4.\ 6)$$

In table 3.6 on page 34 we have brought together the values of these coefficients γ_k and γ'_k. A comparison with tables 3.4 and 3.5 leads to the following conclusions:

(i) Like the expression (5.3. 1), the series (5.4. 3) is a great improvement over the original CM series as far as numerical applicability is concerned.

(ii) For very small x, where $u \propto \beta x$ the series (5.3. 1) converges marginally faster than (5.4. 3), but in this region convergence is no problem anyhow.

(iii) For large positive x, (5.4. 3) is far better than any previous expansion, still converging as $u \rightarrow 1$ though too slowly to be of practical use.

This completes our examination of the isolated atom solution. The series derived in this last section can serve to calculate the function φ accurately (to at least 10 figures) for $1 < x < \infty$, if for the lowest part of this range our summation techniques (appendix 10.2) are applied.

CHAPTER 6 . THE COULSON-MARCH-GILVARRY SOLUTION FOR THE COMPRESSED ATOM

In extending our work to the compressed atom, we have to withdraw the condition that $\psi \to 1$ as $x \to \infty$ which was imposed in the previous chapter; indeed x will not be allowed to become infinite at all. The effect of restricting x to values less than the boundary radius x_0 is studied in this chapter. At the boundary the TF function will have to satisfy a condition different from that for the isolated atom; its consequences will be examined in the next chapter.

6.1 . Formal generalization of the Coulson-March solution

The problems of this and the following chapter are

(i) to find the solution to the TF equation

$$\frac{d^2\varphi}{dx^2} = x^{-\frac{1}{2}} \varphi^{\frac{3}{2}} \qquad (6.1.1)$$

for values of x such that $1 \ll x < x_0$,

imposing the boundary condition

$$\varphi(x_0) = x_0 \varphi'(x_0) \quad ; \qquad (6.1.2)$$

(ii) to cast this solution into a form which gives accurate numerical results when $x \to 1$.

For the present we will ignore the boundary condition; its effect will be discussed in the next chapter.

For large values of x_0 one expects that this solution will not differ dramatically from the CM solution of chapter 5; in particular, we write again

$$\varphi(x) = 144\, x^{-3} \psi(x) \quad . \qquad (6.1.3)$$

whence

$$x^2 \frac{d^2\psi}{dx^2} - 6x \frac{d\psi}{dx} + 12\psi = 12\psi^{\frac{3}{2}} \quad . \qquad (6.1.4)$$

However, as Gilvarry and March [1] first pointed out, if now $\psi(x)$

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1) J.J. Gilvarry & N.H. March, Phys.Rev. 112 (1958) 140-9, referred to as GM.

is written as an expansion in powers x^{λ} the positive root λ_+ of (5.1. 6) can no longer be ignored; since x is restrained to be less than x_0 the terms containing x^{λ_+} no longer diverge at the upper limit of x.

Instead of (5.1. 7) we have to introduce two new independent variables

$$z_- = F_- \; x^{\lambda_-} \qquad \text{and} \qquad z_+ = F_+ \; x^{\lambda_+} \;, \qquad (6.1.\ 5)$$

so that

$$\psi(x) \equiv \psi(z_-, z_+) = \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} e_{k,l} \; z_-^{k} \, z_+^{l} \;. \qquad (6.1.\ 6)$$

With the obvious definitions $\psi_- = \frac{\partial \psi}{\partial z_-}$, $\psi_+ = \frac{\partial \psi}{\partial z_+}$,... etc., the differential equation satisfied by $\psi(z_-, z_+)$ is written as

$$\mu z_-^{2} \psi_{--} - 2 z_- z_+ \psi_{-+} + \mu^{-1} z_+^{2} \psi_{++} + z_- \psi_- + z_+ \psi_+ + 2\psi = 2\psi^{\frac{3}{2}} . \qquad (6.1.\ 7)$$

Here μ is defined as in (5.1. 8). In (6.1. 5) we have introduced two arbitrary parameters F_- and F_+ . They will be determined later by the boundary condition (6.1. 2) and by matching (6.1. 3) to the Baker solution at $x = 1$. By choosing in (6.1. 6) $e_{1,0} = -1$ and $e_{0,1} = 1$ we ensure that for the TF atom the parameters F_- and F_+ are positive. With the help of (6.1. 7) one derives

$$(\mu k - l + 1)(k - 1 - \mu^{-1} l) \; e_{k,l} = 2 \left(\tilde{e}_{k,l} - \tfrac{3}{2} \, e_{k,l} \right) ; \qquad (6.1.\ 8)$$

this recurrence relation, where $\tilde{e}_{k,l}$ has its usual meaning, easily yields the values of $e_{k,l}$ as listed in table 3.7 on page 37. We note that the coefficients $e_{k,0}$ are identical with the e_k of the previous chapter.

At a glance one sees that the series (6.1. 6) is unsuitable for numerical application unless z_- is extremely small. Therefore we study the coefficients $e_{k,l}$ to deduce from them which transformation could cast the function ψ into a more convenient form.

6.2 . **Examination of the CMG series and the transformation of variables suggested by it**

From the previous chapter we know already that the coefficients $e_{4,0} = e_4$ behave like those in the expansion of

$$(1+\beta z_-)^{-4} \qquad \text{with } \beta = .25076\ 23787\ 165016 \quad (6.2.\ 1)$$

A numerical analysis of the coefficients $e_{4,\ell}$ with ℓ fixed, along the lines of section 4.2, shows that they behave like those in the expansion of $(1+\beta z_-)^{-4+10\ell}$, with the same value for β. (6.2. 2)

This behaviour is confirmed by the approximation (cf. section 5.2) of putting $\mu = 0.1$ in (6.1. 7); an exact solution of this equation is

$$\psi_{0.1}(z_-, z_+) = (1+\beta z_-)^{-4}\, f\left[z_+ (1+\beta z_-)^{10}\right] , \qquad (6.2.\ 3)$$

where $f(v)$ is the solution of

$$10\, v^2 f''(v) + v f'(v) + 2 f(v) = 2 f^{\frac{3}{2}}(v) . \qquad (6.2.\ 4)$$

The equations (5.2. 6) and (6.2. 4) bear similar relations to (6.1.7) when $\mu = 0.1$: they can be obtained from it by suppressing the dependence of $\psi_{0,1}$ on z_- or z_+ respectively.

In section 5.4 we already saw the advantage of the transformation $u = \beta z_- / (1+\beta z_-)$ in treating the $(1+\beta z_-)^{-4}$ singularity. A second such transformation is suggested by (6.2. 2/3), which leads to $v = z_+ (1+\beta z_-)^{10}$. Explicitly we write

$$u = \frac{\beta z_-}{1+\beta z_-} , \qquad \beta z_- = \frac{u}{1-u} ; \qquad (6.2.\ 5)$$

$$v = z_+ (1+\beta z_-)^{10} , \qquad z_+ = v (1-u)^{10} \qquad (6.2.\ 6)$$

The differential operator $x \frac{\partial}{\partial x}$ is then recast in the form

$$x \frac{\partial}{\partial x} \longrightarrow \lambda_- (1-u) u \frac{\partial}{\partial u} + (\lambda_+ + 10\lambda_- u) v \frac{\partial}{\partial v} , \qquad (6.2.\ 7)$$

whence the differential equation for $\psi(u, v)$ becomes

$$\mu(1-u)^2u^2\psi_{uu} - 2(1-u)(1-10\mu u)\,uv\,\psi_{uv} + \mu^{-1}(1-10\mu u)^2v^2\psi_{vv}$$
$$+ (1-u)(1-2\mu u)u\psi_u + (1-10u+90\mu u^2)v\psi_v + 2\psi = 2\psi^{\frac{3}{2}} . \quad (6.2.8)$$

Expanding ψ as a double power series we write

$$\psi(x) = \psi(u,v) = \sum_{k=0}^{\infty}\sum_{l=0}^{\infty} \gamma_{k,l}\, u^k v^l \quad ; \quad \gamma_{1,0} = -\frac{1}{\beta} \, , \; \gamma_{0,1} = 1 \, ; \quad (6.2.9)$$

and substitution in (6.2. 8) yields the recursion relation

$$(vk-l+1)(k-1-\mu^{-1}l)\gamma_{k,l} = (k-10l-1)(1-2l+2\mu(k-1))\gamma_{k-1,l}$$
$$-\mu(k-10l-1)(k-10l-2)\gamma_{k-2,l} + 2(\tilde{\gamma}_{k,l} - \tfrac{3}{2}\gamma_{k,l}) . \quad (6.2.10)$$

As is readily seen from the values collected in table 3.8 on page 38 the coefficients $\gamma_{k,l}$ are markedly better from a numerical point of view than the original coefficients $c_{k,l}$. This makes it worthwhile to adopt this formulation in terms of u and v in spite of the complicated form of the equations.

In order to improve still more on the accuracy of numerical calculations, we can make use of the regular behaviour which the $\gamma_{k,l}$ exhibit in their turn: the next section is devoted to the study of these coefficients.

6.3 . Analysis of the expansions in the transformed variables

If we want to calculate $\psi(x)$ for a particular value of x , we must determine z_- and z_+ according to (6.1. 5), then find from them u and v by (6.2. 5/6) and finally insert these values into

$$\psi(x) = \psi(u,v) = \sum_{k,l=0}^{\infty} \gamma_{k,l}\, u^k v^l \quad . \quad (6.3.1)$$

In general the summation (6.3. 1) will be carried out by summing first over one of the indices k or l , then over the other. Explicitly, one can write

either $$\psi_k(v) = \sum_{l=0}^{\infty} \gamma_{k,l}\, v^l \, , \; \psi(u,v) = \sum_{k=0}^{\infty} u^k \psi_k(v) \, , \quad (6.3.2)$$

or $$ {}_\ell\psi(u) = \sum_{k=0}^{\infty} \gamma_{k,\ell}\, u^k \;, \quad \psi(u,v) = \sum_{\ell=0}^{\infty} {}_\ell\psi(u)\, v^\ell . \qquad (6.3.3) $$

The order in which the summations are performed is chosen according to the magnitudes of u and v in each particular case.

In the following we will study the coefficients $\gamma_{k,\ell}$, first considered as the expansion coefficients of functions $\psi_k(v)$ with k fixed, and then considered as the expansion coefficients of functions ${}_\ell\psi(u)$ with ℓ fixed. It will be shown how in either case one can reach a higher numerical accuracy in the summations than would be possible in a straightforward summing of the power series expansions.

6.31

First, let us examine the case represented by equations (6.3.2). By means of the methods of section 4.2 the late coefficients of the expansion of $\psi_k(v)$ are found to behave like those of

$$ \left(1 - \frac{v}{v_x}\right)^{\frac{7}{2}-k} \;; \qquad -v_x^{-1} = 0.9614 \quad . \qquad (6.3.4) $$

This is immediately recognized as similar in type to what was found in section 4.3 for the Baker series. Therefore we set up differential equations for ψ_k and try to deduce (6.3.4) from them, as was done there. For ψ_0,

$$ \mu^{-1} v^2 \psi_0''(v) + v\,\psi_0'(v) + 2\psi_0(v) = 2\psi_0^{\frac{3}{2}}(v) . \qquad (6.3.5) $$

As in the Baker case, ψ_0 is a monotonic increasing function of v, having a simple zero at $v_x = -1.0401\ 80657\ 386153$. (6.3.6)
Thus $-v_x^{-1} = .96137\ 14626\ 388822$, which replaces the estimate (6.3.4). Again, ψ_0 contains contributions of the type $(1 - v/v_x)^{\frac{3}{2}+\beta}$, $\beta = 0, 1, \ldots$.

For general k we find the differential equation

$$ \begin{aligned} &\mu^{-1} v^2 \psi_k'' + (1-2k)\, v\,\psi_k' + \left[2 + k + \mu k(k-1)\right]\psi_k \\ &\quad - 20 v^2 \psi_{k-1}'' + 2\left[-6 + k + 10\mu\,(k-1)\right] v\,\psi_{k-1}' - (k-1)\left[1 + 2\mu(k-1)\right]\psi_{k-1} \\ &\quad + 100\mu v^2 \psi_{k-2}'' + 10\mu(13-2k)\, v\,\psi_{k-2}' + \mu(k-1)(k-2)\psi_{k-2} = 2\psi_k . \end{aligned} \qquad (6.3.7) $$

where

$$\tilde{\psi}_k(v) = \sum_{l=0}^{\infty} \tilde{\gamma}_{k,l}\, v^l \; ; \quad \psi^{\frac{3}{2}}(u,v) = \sum_{k=0}^{\infty} u^k \tilde{\psi}_k(v) . \qquad (6.3.8)$$

This system of equations, though considerably more complicated than that for the Baker functions φ_s, has solutions which show the same qualitative behaviour. Thus here too $\psi_k(v)$ contains contributions of the form

$$\left(1 - \frac{v}{v_2}\right)^{\frac{7}{2}-k+p} , \quad p = 0, 1, 2, \ldots , \qquad (6.3.9)$$

thereby confirming (6.3.4) once more. Since the method (i) of section 4.4 (that of subtracting the contributions (6.3.9) multiplied by appropriate coefficients) does not lead to large enough improvements, we need not go through an analysis to determine the magnitude of these coefficients. For $k \geq r$ we can apply method (ii) of section 4.4, writing

$$\psi_k(v) = \left(1 - \frac{v}{v_2}\right)^{\frac{7}{2}-k} \bar{\psi}_k(v) , \qquad (6.3.10)$$

where the expansion coefficients of $\bar{\psi}_k(v)$ are much smaller than $\gamma_{k,l}$.

In chapter 7 the values of higher derivatives

$$\psi_k^{(m)}(v) = \frac{\partial^m \psi_k}{\partial v^m} , \qquad (6.3.11)$$

calculated for a particular value of v, will also be needed. These can not be evaluated satisfactorily by formal differentiation of the expansions (6.3.2), since the resulting expansions converge very slowly, if at all. Fortunately equation (6.3.7) can be invoked to calculate $\psi_k^{(m)}$ for any m by differentiating the equation $(m-2)$ times; in this manner $\psi_k^{(m)}$ can be calculated from a knowledge of $\psi_k^{(0)}$ and $\psi_k^{(1)}$ only. The latter quantities are obtained from the series expansions, where necessary supplemented by (6.3.10).

Manual calculation along these lines would seem prove impossible for all but the lowest values of k and m. However, the whole process of evaluating the required $\psi_k^{(m)}$ can be formulated

recursively by the application of suitable algorithms to express $\tilde{\psi}_k$ in terms of ψ_k (appendix 10.33) and to express derivatives of $\psi_0^{\frac{3}{2}}$ and ψ_0^{-1} in terms of $\psi_0^{(m)}$ (appendix 10.34). Thus once (6.3. 2) has been summed to yield $\psi_k^{(0)}$ and $\psi_k^{(1)}$, the remainder of the calculation was carried out on the IBM 1620 digital computer.

6.32 .

Let us now turn our attention to the functions $_\ell\psi(u)$ of equation (6.3. 3). To show clearly the difference in behaviour as compared with previously encountered general types, in table 6.1 we have listed a larger number of the coefficients $\gamma_{k,\ell}$ for $\ell = 0, 1, 2, 3$. One immediately notices the striking phenomenon that for certain values of k the coefficients suddenly become large, to drop back again to small values with increasing k. The following argument shows the origin of this phenomenon and - more important - allows us to infer the value of k at which it ceases.

Since ψ is almost behaving like $(1-u)^4$ any large coefficients are expected to occur in groups of at least 5, bearing ratios to each other of roughly 1 : -4 : 6 : -4 : 1 ; an example is formed by the sequence $\gamma_{11,1}$ ..... $\gamma_{15,1}$. To see this more clearly, let us remove the $(1-u)^4$ dependence and examine $\chi(u,v)$, where

$$\psi(u,v) = (1-u)^4\,\chi(u,v) \quad . \tag{6.3.12}$$

Furthermore, as in section 5.2 we take the approximation $\nu = 0.1$ for which the results are particularly simple. Then,

$$\tfrac{1}{10}\,u^2\,{}_\ell\chi'' + (1-2\ell)\,u\,{}_\ell\chi' + (10\ell^2 - 9\ell + 2)\,{}_\ell\chi = 2\,{}_\ell\tilde{\chi} \quad , \tag{6.3.13}$$

with

$$\chi_{0,1}(u,v) = \sum_{\ell=0}^{\infty} {}_\ell\chi(u)\,v^\ell \quad , \quad \chi_{0,1}^{\frac{3}{2}}(u,v) = \sum_{\ell=0}^{\infty} {}_\ell\tilde{\chi}(u)\,v^\ell \quad . \tag{6.3.14}$$

For $\ell = 0$, there is a trivial solution ${}_0\chi(u) \equiv 1$; then one writes

Table 6.1

Some coefficients $\gamma_{k,\ell}$ as illustration of section 6.32

k	$\gamma_{k,0}$	$\gamma_{k,1}$	$\gamma_{k,2}$	$\gamma_{k,3}$
0	.1000000000E+01	.1000000000E+01	.3548671274E-01	-.1150085184E-02
1	-.3987839026E+01	-.4018241462E+01	-.1441985209E-00	.4693659762E-02
2	.5962540743E+01	.6052796232E+01	.2192192514E-00	-.7181800058E-02
3	-.3961414582E+01	-.4051289251E+01	-.1479911199E-00	.4879531222E-02
4	.9866806638E-00	.1016554064E+01	.3734695128E-01	-.1245792551E-02
5	.8620582631E-05	-.1139144916E-03	-.1387233985E-03	-.5992362473E-05
6	.5916402028E-05	-.2252141764E-03	-.3472274085E-03	-.1679204601E-04
7	.4169917351E-05	-.4980150664E-03	-.1037962904E-02	-.5573919158E-04
8	.3007560046E-05	-.1296753074E-02	-.4094314798E-02	-.2424558012E-03
9	.2213474017E-05	-.4381834484E-02	-.2738234809E-01	-.1776282210E-02
10	.1658377770E-05	-.2457748510E-01	-.2488742048E+01	-.1756752602E-00
11	.1262372414E-05	-.1820726001E+01	.1361044679E+02	.1038378238E+01
12	.9746910724E-06	.7789624155E+01	-.2873512806E+02	-.2353871685E+01
13	.7622718719E-06	-.1206065448E+02	.2998232204E+02	.2621419704E+01
14	.6031025381E-06	.8202986023E+01	-.1555060995E+02	-.1443748336E+01
15	.4822329763E-06	-.2079930662E+01	.3214406100E+01	.3153223679E-00
16	.3893248326E-06	-.4467062416E-05	-.3821055865E-03	-.2517650015E-03
17	.3171106111E-06	-.3698332723E-05	-.9012436553E-03	-.5704898698E-03
18	.2604043058E-06	-.3005767023E-05	-.2514843537E-02	-.1395898095E-02
19	.2154539338E-06	-.2427284223E-05	-.9145555898E-02	-.2484797351E-02
20	.1795103536E-06	-.1959342194E-05	-.5469498414E-01	.2674062318E-00
21	.1505354706E-06	-.1585945206E-05	-.2360294821E+01	-.4711619595E+01
22	.1270018200E-06	-.1289368099E-05	.1319880308E+02	.2059801287E+02
23	.1077530076E-06	-.1053775753E-05	-.2736820490E+02	-.4032882547E+02
24	.9190528127E-07	-.8661114391E-06	.2768315565E+02	.4064164071E+02
25	.7877728144E-07	-.7159928032E-06	-.1382569141E+02	-.2069780596E+02
26	.6783934328E-07	-.5953042434E-06	.2740334897E+01	.4234496769E+01
27	.5867652770E-07	-.4977490225E-06	-.4839819311E-05	-.1885728583E-02
28	.5096139925E-07	-.4184518636E-06	-.3621420950E-05	-.5368807893E-02
29	.4443379692E-07	-.3536342836E-06	-.2723396357E-05	-.1989283556E-01
30	.3888567131E-07	-.3003594965E-06	-.2064797842E-05	-.1194435854E-00
31	.3414962651E-07	-.2563358693E-06	-.1580340320E-05	-.3715505267E+01
32	.3009019475E-07	-.2197669319E-06	-.1221547954E-05	.2494384190E+02
33	.2659714355E-07	-.1892373588E-06	-.9535335294E-06	-.6157307173E+02
34	.2358030640E-07	-.1636263390E-06	-.7514527919E-06	.7763312949E+02
35	.2096556398E-07	-.1420416492E-06	-.5976280515E-06	-.5369851385E+02
36	.1869170032E-07	-.1237693346E-06	-.4794292602E-06	.1944677867E+02
37	.1670792881E-07	-.1082351589E-06	-.3877723443E-06	-.2888369486E+01
38	.1497193438E-07	-.9497494130E-07	-.3160712685E-06	-.5816557103E-05
39	.1344831575E-07	-.8361162887E-07	-.2595098593E-06	-.4243464022E-05
40	.1210733964E-07	-.7383748828E-07	-.2145350348E-06	-.3137599640E-05

$$ {}_{\ell}\tilde{\chi} = \tfrac{3}{2}\ {}_{\ell}\chi + [\text{function of } {}_{1}\chi, \ldots, {}_{\ell-1}\chi] \ . \qquad (6.3.15) $$

This means that (6.3.13) becomes a linear inhomogeneous equation, whose homogeneous part can be written as

$$ \tfrac{1}{10}\, u^2\, {}_{\ell}\chi'' + (1-2\ell)\, u\, {}_{\ell}\chi' + (\ell-1)(10\ell+1)\, {}_{\ell}\chi = 0 \ . \qquad (6.3.16) $$

Thus besides a particular solution determined by the source term (in square brackets in (6.3.15)) ${}_{\ell}\chi$ contains terms like $u^{10\ell-10}$ and $u^{10\ell+1}$, and can be written

$$ {}_{\ell}\chi = \alpha_{\ell}\ u^{10\ell-10} + \beta_{\ell}\ u^{10\ell+1} + \text{particular soln.} \ . \qquad (6.3.17) $$

For $\mu = 0.1$ the first few ${}_{\ell}\chi$ are therefore

$$ \left.\begin{aligned} {}_{0}\chi &= 1 \\ {}_{1}\chi &= 1 + \beta_1\, u^{11} \qquad (\alpha_1 = 1) \\ {}_{2}\chi &= \tfrac{1}{28} + \alpha_2\, u^{10} - \tfrac{3}{2}\beta_1\, u^{11} + \beta_2\, u^{21} + \tfrac{5}{8}\beta_1^{\,2}\, u^{22} \\ &\ldots\ldots \end{aligned}\right\} \qquad (6.3.18) $$

In reality $\mu \neq 0.1$ and thus α_{ℓ} and β_{ℓ} are not entirely arbitrary; but it seems clear that there is scope for anomalously large values of the coefficients. With ${}_{\ell}\psi = (1-u)^4\, {}_{\ell}\chi$ the large values of $\gamma_{k,\ell}$ occur at the k-values predicted by (6.3.17/18). Also, if we take $\beta_1 = \gamma_{11,1}$, the magnitudes of $\gamma_{11,2}$, $\gamma_{11,3}$, $\gamma_{22,2}$, etc. are explained quite well by (6.3.18).

Although we have not found any satisfactory way of removing these anomalously large values, this examination specifies which terms are affected. In ${}_{\ell}\chi$ these large coefficients occur for $k = 10, 11; 20, 21, 22; \ldots\ldots; 10\ell+1, \ldots, 11\ell$, but not for $k > 11\ell$. This means that in ${}_{\ell}\psi$ no large values occur for $k > 11\ell+4$ as is confirmed by the values in table 6.1. Therefore if we plan the

summation (6.3. 3) to go well beyond $f_{\ell+4,\ell}$ it can be safely assumed that we obtain a reasonable accuracy; typically, u will not be larger than $u \approx .77$.

It is disappointing to have to leave this intriguing problem; however, we feel that the small extra accuracy which might possibly be gained does not warrant expenditure of more time and effort.

As in section 6.31 , we will need the higher derivatives ${}_\ell\psi^{(m)}(u)$. These can be calculated in exactly the same fashion as indicated there; instead of (6.3. 7) ${}_\ell\psi$ has to satisfy

$$\nu(1-u)^2u^2\,{}_\ell\psi'' + \left[(1-2\ell)+2\mu(10\ell-1)\right](1-u)u\,{}_\ell\psi' + \left[2+\ell+\mu^{-1}\ell(\ell-1)-10\ell(2\ell-1)u+10\mu\ell(10\ell-1)u^2\right]{}_\ell\psi = 2\,{}_\ell\tilde{\psi} \quad (6.3.19)$$

where

$${}_\ell\tilde{\psi}(u) = \sum_{k=0}^{\infty} \tilde{f}_{k,\ell}\,u^k \quad ; \quad \psi^{\frac{3}{2}}(u,v) = \sum_{\ell=0}^{\infty} {}_\ell\tilde{\psi}(u)\,v^\ell . \quad (6.3.20)$$

This completes our analysis of the CMG function; in the next chapter we will show how to determine the parameters F_- and F_+ , and with them the entire TF function of the compressed atom, from the boundary condition at x_0 (6.1. 3) and by joining the CMG solution to the Baker solution of chapter 4 at $x = 1$.

CHAPTER 7 . DETERMINATION OF THE INTEGRATION CONSTANTS FROM THE BOUNDARY CONDITIONS

In chapter 4 we derived a functional form, the Baker solution, valid for $0 \leq x \leq 1$, satisfying the boundary condition at $x = 0$ and containing one parameter $\mathcal{B}$ (cf. equation (4.1. 3)). In chapter 6 we obtained another form, the CMG solution, valid for $1 \leq x \leq x_0$, and containing the two parameters F_- and F_+ (cf. equation (6.1. 5)). From these two a solution covering all values of x can be constructed; if $\mathcal{B}$, F_- and F_+ are determined from the boundary condition at x_0 and from conditions of continuity at $x = 1$, this solution will satisfy the TF boundary conditions. As a result of this procedure we find the three parameters as function of the boundary radius x_0. In the first section of this chapter the proper functional form of this dependence is established; in the second a valuable relation between these functions is derived; and in the last section we calculate the numerical coefficients in them.

7.1 . Expected functional dependence of the parameters on the boundary radius

Our task is to find expressions for the dependence of the initial slope $\mathcal{B} \equiv \varphi'(0)$ and of the CMG parameters F_- and F_+ of (6.1. 5) on the boundary radius x_0 . To these we add the value of φ at x_0, occurring in the expressions for energy and pressure of section 1.2 , and given by

$$\varphi^0 \equiv \varphi(x_0) = 144\, x_0^{-3}\, \psi^0 \quad ; \quad \psi^0 \equiv \psi(x_0). \tag{7.1. 1}$$

These functional dependences must be determined from the condition of continuity at $x = 1$:

$$\varphi_{Baker}(1) = \varphi_{CMG}(1) \quad , \quad \varphi'_{Baker}(1) = \varphi'_{CMG}(1) \, , \tag{7.1. 2}$$

and the boundary condition at x_0 :

$$\varphi_{CMG}(x_0) = x_0\, \varphi'_{CMG}(x_0) \, . \tag{7.1. 3}$$

These relations will be our guide as to how to express our parameters in terms of x_0. We want an expansion in terms of a parameter which becomes small as x_0 becomes large, so that the isolated-atom values are obtained as $x_0 \to \infty$. It transpires that two such expansion parameters must be introduced.

First let us concentrate on the condition (7.1. 3) and on $\psi^\circ(x_0)$. The relation (7.1. 3) leads to a functional dependence between $F_-(x_0)$ and $F_+(x_0)$. However, it is easier to write this as a relation between the values of u and v of (6.2. 5/6) for $x = x_0$:

$$u_0(x_0) \equiv u(x=x_0) = \frac{\beta F_-(x_0)\, x_0^{\lambda_-}}{1+\beta F_-(x_0)\, x_0^{\lambda_-}} \quad ; \tag{7.1. 4}$$

$$v_0(x_0) \equiv v(x=x_0) = F_+(x_0)\, x_0^{\lambda_+}\, (1+\beta F_-(x_0)\, x_0^{\lambda_-})^{10} . \tag{7.1. 5}$$

Any relation between u_0 and v_0 is of course equivalent to a relation between F_- and F_+. For $x_0 \to \infty$ all functions of x_0 are expected to tend to their isolated-atom values; thus, $u_0 = O(x_0^{\lambda_-})$ as $x_0 \to \infty$. Since it is easily checked that $v_0 = O(1)$ as $x_0 \to \infty$, u_0 is the obvious choice as expansion parameter. We write tentatively

$$v_0 = v_0(u_0) = \sum_{i=0}^{\infty} \sigma_i\, u_0^{\,i} \quad ; \tag{7.1. 6}$$

$$\psi^\circ = \psi^\circ(u_0) = \sum_{i=0}^{\infty} \pi_i\, u_0^{\,i} \quad . \tag{7.1. 7}$$

Similarly, the conditions (7.1. 2) suggest the appropriate expansion parameter: two equations are found containing $\mathcal{B}$ and

$$u_1(x_0) \equiv u(x=1) = \frac{\beta F_-(x_0)}{1+\beta F_-(x_0)} \quad ; \tag{7.1. 8}$$

$$v_1(x_0) \equiv v(x=1) = F_+(x_0)\, (1+\beta F_-(x_0))^{10} . \tag{7.1. 9}$$

On inspection we see that as $x_0 \to \infty$, $\mathcal{B} = O(1)$ and $u_1 = O(1)$, while $v_1 = O(x_0^{-\lambda_+})$. Thus expansions are expected of the form:

$$\mathcal{B} = \mathcal{B}(v_1) = \sum_{i=0}^{\infty} \mathcal{B}_i\, v_1^{\,i} \quad ; \tag{7.1.10}$$

$$u_1 = u_1(v_1) = \sum_{i=0}^{\infty} \tau_i\, v_1^{\,i} \quad . \tag{7.1.11}$$

For arbitrary x, $u(x)$ and $v(x)$ can be written in terms of u_1 and v_0 instead of F_- and F_+:

$$u(x) = \frac{u_1 x^{\lambda_-}}{1-u_1+u_1 x^{\lambda_-}} \quad ; \quad v(x) = v_0 \left(\frac{x}{x_0}\right)^{\lambda_+} \left(\frac{1-u_1+u_1 x^{\lambda_-}}{1-u_1+u_1 x_0^{\lambda_-}} \right)^{10} . \quad (7.1.12)$$

From the conditions (7.1. 2/3) the coefficients of (7.1. 6/11) can be derived if u_0 and v_1 are connected with u_1 and v_0 by

$$u_0 = \frac{u_1 x_0^{\lambda_-}}{1-u_1+u_1 x_0^{\lambda_-}} \quad ; \quad v_1 = v_0 x_0^{-\lambda_+} (1-u_1+u_1 x_0^{\lambda_-})^{-10} . \quad (7.1.13)$$

We could try to convert the expressions suggested above into forms giving explicitly the dependence of F_- and F_+ on x_0. However, there is no reason to prefer the latter as parameters over u_1 and v_0, or indeed any other pair, apart from the historical fact that they were introduced first. Also, (7.1. 6/11) are functions of a single variable, while the relations (7.1.13) connect these by analytic expressions; expansions of F_- and F_+, on the other hand, would have to contain powers of both $x_0^{\lambda_-}$ and $x_0^{-\lambda_+}$. This is easily seen if one tries to write down explicit forms for such expansions. The fact that u_1 and v_0 have to be found recursively is no great impediment: starting from the isolated-atom value of u_1, two or three iterations normally suffice to arrive at stable values.

These expansions must be compared with those suggested by GM [1], who assumed that F_-, $F_+ x_0^{\lambda_+}$, ψ^0 and $(B-B_0)x_0^{\lambda_+}$ could be written as expansions in $x_0^{\lambda_-}$ only. There are two reasons apparent why they did not observe inconsistencies resulting from this assumption: the first is that they did not actually perform the suggested calculations beyond the first few terms, and thus could not find anything amiss since non-zero coefficients of $x_0^{-\lambda_+}$ only occur beyond where they stopped. The second reason is that they proposed the use of numerical values for the TF function, instead of our matching process at $x=1$. Thus, they would have got the "best possible fit" in the framework of their assumed form if they had actually carried through the proposed calculation, and would not necessarily have noticed the incompleteness of the assumed forms.

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1) J.J. Gilvarry & N.H. March, Phys.Rev. 112 (1958) 140-9.

7.2 . The pressure-energy relation in terms of the parameters

It is very illuminating to insert the expansions obtained in the previous section into the relation between pressure, energy and atomic volume $p = -\partial E/\partial v$, which in terms of x_0 can be written

$$p v = -\frac{1}{3} x_0 \frac{\partial E}{\partial x_0} \quad . \tag{7.2. 1}$$

With the help of (1.2. 14/15) this can be re-expressed in terms of φ° and x_0 as

$$\frac{\partial B}{\partial x_0} = - x_0^{-\frac{1}{2}} (\varphi^\circ)^{\frac{3}{2}} \left[1 + \frac{1}{3} \frac{x_0}{\varphi^\circ} \frac{d\varphi^\circ}{dx_0} \right] . \tag{7.2. 2}$$

Here we must remember when taking the derivatives that φ° depends on x_0 both explicitly via the argument, and implicitly via u_1 and v_0 . With (7.1. 1)

$$\frac{\partial B}{\partial x_0} = - 82944\, x_0^{-7} (\psi^\circ)^{\frac{9}{2}} \frac{d\psi^\circ}{dx_0} \quad . \tag{7.2. 3}$$

Let us now substitute the expansions (7.1. 6/7/10/11) into this relation. Some manipulation and application of the relations (7.1.13) leads to

$$\frac{\frac{\partial B}{\partial v_1}}{(1-u_1)^8 \left[\mu u_1 (1-u_1) + (1-10\mu u_1) v_1 \frac{du_1}{dv_1} \right]} = \frac{- 82944 (\psi^\circ)^{\frac{9}{2}} \frac{d\psi^\circ}{du_0}}{(1-u_0)^8 \left[(1-10\mu u_0) v_0 + \mu (1-u_0) u_0 \frac{dv_0}{du_0} \right]} . \tag{7.2. 4}$$

With our assumptions the left-hand side of this equation is a function only of v_1, the right-hand side only of u_0 ; thus we expect both to be equal to a constant independent of x_0 .

This relation provides a check on the calculations of the next section. On either side of the equation, expansion in powers of the appropriate variable must give coefficients for numerator and denominator that have a constant ratio: this ratio must be equal for the two different sides.

7.3 . **Numerical values**

Following the ideas set out in the first section of this chapter the determination of the actual values of the expansion coefficients will now be outlined. We start with the expansions of v_0 and ψ° (7.1. 6/7). In terms of the function ψ (6.1. 3) and the variables u and v the boundary condition (7.1. 3) can be written, applying (6.2. 7), as

$$0 = 4\,\psi(u_0,v_0) - \lambda_-(1-u_0)\,u_0\,\psi_u(u_0,v_0) - (\lambda_+ + 10\lambda_-\,u_0)\,v_0\,\psi_v(u_0,v_0). \quad (7.3.\ 1)$$

With the help of the functions $\psi_k(v)$ of (6.3. 2) this reduces to a very simple form: let

$$\psi_k^*(v) = (4 - k\lambda_-)\,\psi_k(v) + (k-1)\lambda_-\,\psi_{k-1}(v) - \lambda_+ v\,\psi_k'(v) - 10\lambda_-\,v\,\psi_{k-1}'(v) \quad ; \quad (7.3.\ 2)$$

then (7.3. 1) goes into

$$0 = \sum_{k=0}^{\infty} u_0^{\,k}\,\psi_k^*(v_0) \quad . \quad (7.3.\ 3)$$

Similarly ψ° can be written

$$\psi^\circ = \sum_{k=0}^{\infty} u_0^{\,k}\,\psi_k(v_0) \quad . \quad (7.3.\ 4)$$

Now by substituting (7.1. 6) for v_0 it is possible to write these two expressions as expansions in u_0 only; the method is completely described in appendix 10.35. Equation (7.3. 3) then takes the form

$$0 = \sum_{i=0}^{\infty} \pi_i^*\,u_0^{\,i} \quad , \quad (7.3.\ 5)$$

where the coefficients π_i^* depend on σ_0 , ..., σ_i and on the derivatives $\psi_k^{*(m)}(\sigma_0)$ (cf. 6.3.11). The latter are calculated by the method outlined in section 6.31. By successively putting $\pi_i^* = 0$, $i = 0, 1, 2, \ldots$ the values of σ_i can be obtained. The value of σ_0 itself is the root of

$$0 = \psi_0^* = 4\psi_0 - \lambda_+ v\,\psi_0' \quad ; \quad \sigma_0 = .963651735137592\ldots \quad (7.3.\ 6)$$

Once the values of σ_i are known, it is quite simple to find the coefficients π_i of (7.1. 7); from (7.3. 4) we see that they bear the same functional relationship to $\psi_4^{(m)}(\sigma_0)$ as π_i^* to $\psi^{*}{}_4^{(m)}(\sigma_0)$.

In table 3.10 on page 40 we have collected values of σ_i (column 2) and π_i (column 3), together with the expansion of $(1-\mu_0)^{-4}\psi^{\circ}(\mu_0)$ (column 4) which because of its smoothness is very suitable for numerical calculations. With the help of these values we have also formed the expansions of numerator and denominator of the r.h.s of (7.2. 4): as expected, corresponding coefficients in these two expansions have a common ratio, which has the value

$$1.8303\ 56455\ 21 \times 10^{6} \quad , \qquad (7.3.\ 7)$$

being constant to at least 10 significant figures for the first 14 terms. This illustrates the accuracy of our numerical values, since the relation (7.2. 4) is derived in a manner entirely independent of the calculation above.

Next let us determine the expansions of $\mathcal{B}$ and μ, (7.1. 10/11). Obviously $\mathcal{B}_0$ and τ_0 are given by their isolated-atom values (3.3. 4):

$$\mathcal{B}_0 = -1.5880\ 710226 \quad ; \quad \tau_0 = .76893\ 89731 \quad . \qquad (7.3.\ 8)$$

According to the results of chapter 4

$$\varphi_{Baker}(1) = \sum_{s=0}^{\infty} b_s\, \mathcal{B}^s \quad ; \quad \varphi'_{Baker}(1) = \sum_{s=0}^{\infty} b_s'\, \mathcal{B}^s \quad . \qquad (7.3.\ 9)$$

where the coefficients b_s and b_s' have to be evaluated at $x=1$ in accordance with (4.4. 3/5). By a method similar to that of appendix 10.35 one can write this under substitution of (7.1.10) as

$$\varphi_{Baker}(1) = \sum_{i=0}^{\infty} g_i\, \mu_i^{\,i} \quad ; \quad \varphi'_{Baker}(1) = \sum_{i=0}^{\infty} g_i'\, \nu_i^{\,i} \quad . \qquad (7.3.10)$$

Here g_i and g_i' are functions of $\mathcal{B}_i$ and of the derivatives $\left[\partial^k \varphi_{Baker}(1)/\partial \mathcal{B}^k\right]_{\mathcal{B}=\mathcal{B}_0}$ and $\left[\partial^k \varphi'_{Baker}(1)/\partial \mathcal{B}^k\right]_{\mathcal{B}=\mathcal{B}_0}$ which can be calculated from (7.3. 9). On the other hand, by chapter 6,

$$\varphi_{end}(1) = 144 \sum_{l=0}^{\infty} {}_l\psi(u_1)\, v_1^{\,l} \; ; \; \varphi'_{end}(1) = 144 \sum_{l=0}^{\infty} {}_l\psi^*(u_1)\, v_1^{\,l} \quad (7.3.11)$$

where

$${}_l\psi^*(u) = (-3 + l\lambda_+ + 10 l \lambda_- u)\, {}_l\psi(u) + \lambda_-(1-u)\, u\, {}_l\psi'(u) \; . \quad (7.3.12)$$

Following once more the method of appendix 10.35, substituting (7.1.11) and expanding leads to

$$\varphi_{end}(1) = \sum_{i=0}^{\infty} h_i\, v_1^{\,i} \; ; \; \varphi'_{end} = \sum_{i=0}^{\infty} h'_i\, v_1^{\,i} \; , \quad (7.3.13)$$

where h_i and h'_i depend on τ_i and on resp. ${}_l\psi^{(m)}(\tau_0)$ and ${}_l\psi^{*(m)}(\tau_0)$. The necessary values of these derivatives are calculated by the method indicated in sections 6.31 and 6.32.

The matching conditions (7.1.2) now reduce to the very simple form

$$g_i = h_i \quad ; \quad g'_i = h'_i \quad ; \quad i = 0, 1, 2, \ldots \; . \quad (7.3.14)$$

The zero-order equations ($i=0$) are automatically satisfied by adopting the values (7.3.8); since for $i \geq 1$ the equations are linear in $\mathcal{B}_i$ and τ_i they can be solved in a straightforward manner. In table 3.9 on page 40 we have listed the values of $\mathcal{B}_i$ and τ_i calculated in this way. In this case we have expanded numerator and denominator of the l.h.s. of (7.2.4): again we find that corresponding coefficients in these expansions have a common ratio, with the value

$$1.8303\ 56455\ 19 \times 10^{6} \; . \quad (7.3.15)$$

This agrees excellently with (7.3.7). For the first three coefficients of the expansions the ratio is equal to better than 10 significant figures, for the next two to better than 8 figures. We conclude that the accuracy reached is most satisfactory.

As a check on the applicability and reliability of these expansions we have calculated u_1 and v_0, and from them $\mathcal{B}$ and

Table 7.1

Comparison of our results for $B(x_0)$ and $\varphi^\circ(x_0)$ with those of Latter (ref. 2)

x_0	Latter's work		This work			
	B	φ°	n_{it}	B	φ°	n_{ae}
2.200	-1.4999	.666280	5	-1.4998545	.668874763	3
2.800	-1.5500	.476670	4	-1.5499931	.477204579	3
3.043	-1.5601	.422620	4	-1.5599826	.422950822	3
3.285	-1.5671	.377510	4	-1.5669826	.377706416	3
3.704	-1.5746	.314830	4	-1.5748024	.314867777	4
4.230	-1.5803	.255700	3	-1.5802807	.255725495	4
4.330	-1.5809	.246330	3	-1.5809933	.246344174	4
5.229	-1.5849	.180580	3	-1.5848888	.180588736	4
5.401	-1.5853	.170950	3	-1.5853090	.170947210	4
5.850	-1.5862	.148990	3	-1.5861346	.148996559	5
6.206	-1.5866	.134330	3	-1.5865898	.134338778	5
7.385	-1.5874	.098098	2	-1.5874152	.098100443	5
7.790	-1.5876	.088823	2	-1.5875643	.088822659	5
8.015	-1.5876	.084193	2	-1.5876300	.084192574	5
8.588	-1.5876	.073821	2	-1.5877576	.073824693	6
8.590	-1.5876	.073789	2	-1.5877579	.073791704	6
9.565	-1.5879	.059868	2	-1.5878892	.059869115	6
10.804	-1.5880	.046934	2	-1.5879745	.046934486	6
11.300	-1.5880	.042832	2	-1.5879949	.042833657	7
11.963	-1.5880	.038086	2	-1.5880149	.038086451	7
15.870	-1.5881	.020825	2	-1.5880594	.020824774	8
16.000	-1.5881	.020454	2	-1.5880599	.020454409	8

φ°, for those values x_0 for which Latter [2] calculated the latter two quantities by inward numerical integration. In table 7.1 our results are compared with Latter's. The column labeled n_{it} gives the number of iterations necessary to obtain stable values u, and v_0, that labeled n_{se} the number of reliable significant figures in our results. The expansion for $(1-u_0)^{-4}\psi^\circ(u_0)$ as given in table 3.10 was applied in order to find φ°, supplemented by the techniques for improving convergence described in appendix 10.2. For x_0 as small as 3.7 we still achieve reasonable agreement with Latter; previously reported "accurate" solutions did not reach this precision (cf. also Latter's table, which quotes a number of other authors).

This concludes our consideration of solutions for compressed atoms with large atomic radii. In the next chapter we will expound an entirely different approach, designed to meet the case of small atomic radius, where $x_0 \lesssim 1$ and the above expansion methods fail.

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2) R. Latter, J.Chem.Phys. 24 (1955) 280-92, in part. table III, p. 292.

CHAPTER 8 . THE THOMAS-FERMI-DIRAC EQUATION FOR VERY SMALL ATOMIC RADIUS

When the atomic radius becomes very small ($x_0 \lesssim 1$) the method applied in the previous chapters fails, since the range $0 \leq x \leq x_0$ no longer contains a part where $x >> 1$. In the present chapter we develop a method to deal with this situation: since this method is equally applicable to the TFD equation (section 1.3) we treat this more general case, from which the TF equation and its solution can easily be recovered.

8.1 . An integral equation for the TFD function and its iterative solution

We follow an approach due to March [1], who assumed that $\varphi(x)$ could be expanded as a Taylor series around x_0 . Choosing values for function and derivative satisfying the boundary condition at x_0, he obtained higher derivatives from the differential equation; thus he found the first few terms of a series expressing $\varphi(x)$ with the value of $\varphi(x_0)$ as a parameter. The latter could finally be eliminated by invoking the boundary condition at the origin. Unfortunately divergences appeared after the first two terms. The basic reasons for this, as we will shortly see, are

(i) that the expansion around x_0 can not be written as a power (Taylor) series, since it contains logarithmic contributions in the third and higher orders;

(ii) that in any case the expansion around x_0 can not, in its simplest form, be extended as far as the origin $x = 0$.

Here a method is developed [2] avoiding these pitfalls. First it is convenient to change the independent variable, to simplify notation in a later stage. Writing $x = 3^{\frac{2}{3}} y$ and $\beta_0 = 3^{-\frac{1}{2}} \beta$ changes the basic equation (1.3. 7) into

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1) N.H. March, Proc.Phys.Soc.A 68 (1955) 726-34.

2) P.J. Rijnierse, Proc.Roy.Soc.(London)A 292 (1966) 288-97.

$$\frac{d^2\varphi}{dy^2} = 3y^{-\frac{1}{2}}\left(\varphi^{\frac{1}{3}} + \beta y^{\frac{1}{3}}\right)^3 \quad . \qquad (8.1.\ 1)$$

The boundary conditions $\varphi(0) = 1$ and $\varphi(y_0) = y_0 \left.\frac{d\varphi}{dy}\right|_{y=y_0}$ (8.1. 2) where $y_0 = 3^{-\frac{2}{3}} x_0$, retain the same form in y as they had in x, but it will be necessary to introduce the scale factor $3^{\frac{2}{3}}$ into equations (1.2. 6) and (1.3. 10/11).

Now we essentially follow March [1] in writing

$$\varphi(y_0) = a^2 y_0 \quad , \quad \varphi'(y_0) = a^2 \quad , \qquad (8.1.\ 3)$$

thus satisfying the boundary condition and at the same time introducing a helpful parameter a. (Note that our a is $3^{+\frac{1}{3}}$ times that of March.) Later a and hence $\varphi(y_0)$ will be determined from the boundary condition at $y = 0$.

Making assumptions about the form for $\varphi(y)$ to be expected might prevent us from finding such things as logarithmic contributions unless we realize beforehand that they might occur. To avoid this an iterative approach is adopted which will generate these terms for us. It is essentially based on the idea that successive integration, inserting accurate boundary values, increases accuracy, whereas differentiation decreases it. Therefore (8.1. 1) is integrated twice, substituting (8.1. 3), to yield

$$\varphi'(y) = a^2 + 3\int_{y_0}^{y} z^{-\frac{1}{2}}\left(\varphi^{\frac{1}{3}} + \beta z^{\frac{1}{3}}\right)^3 dz \quad ; \qquad (8.1.\ 4)$$

$$\varphi(y) = a^2 y + 3\int_{y_0}^{y} z^{-\frac{1}{2}}(y-z)\left(\varphi^{\frac{1}{3}} + \beta z^{\frac{1}{3}}\right)^3 dz \quad . \qquad (8.1.\ 5)$$

Given an approximation to φ, φ_n say, an approximation accurate to the next higher order is now obtained from the recurrence relation

$$\varphi_{n+1}(y) = a^2 y + 3\int_{y_0}^{y} z^{-\frac{1}{2}}(y-z)\left[\varphi_n^{\frac{1}{3}}(z) + \beta z^{\frac{1}{3}}\right]^3 dz \quad . \qquad (8.1.\ 6)$$

An appropriate zero-order approximation is immediately suggested by (8.1. 6) itself: we choose $\varphi_0(y) = a^2 y$. This easily yields

the next approximation

$$\varphi_1(y) = a^2 y + \tfrac{1}{2}(a+\beta)^3 (y^3 - 3yy_0^2 + 2y_0^3) . \qquad (8.1.7)$$

The limit $y \to 0$ is of special interest; we see that

$$1 \approx \varphi_1(0) = (a+\beta)^3 y_0^3 , \qquad (8.1.8)$$

which shows that $a \approx y_0^{-1}$, and also that $l \equiv \frac{\beta}{a} \approx \beta y_0$. (8.1.9)

To proceed to the next higher approximation we require an expansion of $\varphi_1^{\frac{1}{2}}$. If $a^2 y$ in (8.1.7) is taken as the leading term in such a multinomial expansion, successive application of (8.1.6) yields terms up to order a^5 inclusive. Then, one stage later than in March's approach, divergences appear. The reason for this is that near the origin $a^2 y \to 0$ and hence in that region we cannot accept $a^2 y$ as the leading term in a multinomial expansion. To rectify this we rewrite (8.1.7) and subsequent approximations in the form

$$\varphi_1(y) = a^2(y+\alpha) + \tfrac{1}{2}a^3(1+l)^3(y^3 - 3yy_0^2) , \qquad (8.1.10)$$

thereby incorporating into the leading term the definitely non-zero quantity

$$\alpha \equiv a(1+l)^3 y_0^3 \qquad (8.1.11)$$

We note that for small y_0 , $\alpha \approx y_0^2$.

With $a^2(y+\alpha)$ as the new leading term in a multinomial expansion, (8.1.6) involves integrals of the general form

$$I_{s,t} = \int_{y_0}^{y} z^s (z+\alpha)^t \, dz \qquad (8.1.12)$$

where s and t are either both integers or both half-odd-integers. The integrated forms contain terms of the types $(z+\alpha)^t$ and $\operatorname{arsinh}(z/\alpha)^{\frac{1}{2}}$. Different expansions for these functions exist, according as $|z/\alpha| > 1$ or < 1 . At the definite lower limit $z = y_0$ this gives no trouble: if $y_0 < 1$, $\alpha/y_0 \approx y_0 \lesssim 1$, and we can expand in rising powers of α/y_0 . For the upper limit $z = y$, however, we cannot form an expansion in this manner; when $y \approx y_0$ the quantity α/y

is less than 1, while for $y \approx 0$ the opposite is true. In fact, this is the root of the divergences occurring in March's theory, and in ours if $a^2 y$ is taken as the leading term in expansions of (8.1. 7): we then automatically obtain expansions in α/y, which, as we now realize, fail in the limit $y \to 0$. Thus $(z+\alpha)^t$ and $\operatorname{arcsinh}(z/\alpha)^{\frac{1}{2}}$ have to be retained in closed form; in the next iteration the latter generates a new type of integral of the form

$$J_{s,t} = \int_{y_0}^{y} z^s (z+\alpha)^t \operatorname{arcsinh}(z/\alpha)^{\frac{1}{2}}\, dz \quad . \tag{8.1.13}$$

This integral does not give rise to new difficulties, at least not to the order of approximation reached by us. The evaluation of $I_{s,t}$ and $J_{s,t}$ is indicated in appendix 10.4.

Proceeding in this way we can obtain better approximations $\varphi_2(y)$, etc. . In the next section the results to fourth order will be presented; also from them expansions for pressure and energy to fifth order in y_0 will be deduced.

8.2 . The fourth-order iterated solution and the results obtained with it

Proceeding as indicated in the previous section, we have obtained, after complex but unexciting calculations, the fourth-order approximation:

$$\begin{aligned}
\varphi(y) = {} & a^2(y+\alpha) + \tfrac{1}{2} a^3 \Big[(1+3b^2) y^{\frac{5}{2}} (y+\alpha)^{\frac{1}{2}} + (3b+b^3) y^3 - 3(1+b)^3 y y_0^2 \Big] \\
& + \tfrac{1}{80} a^4 \Big[9(1+10b^2+5b^4) y^5 + 9(5b+10b^3+b^5) y^{\frac{9}{2}} (y+\alpha)^{\frac{1}{2}} \\
& \quad - 90(1+b)^3 y_0^2 \big\{ (1+b^2) y^{\frac{5}{2}} (y+\alpha)^{\frac{1}{2}} + 2b y^3 \big\} \\
& \quad + 40(1+b)^3 y_0^3 \big\{ (4+3b^2) y^{\frac{3}{2}} (y+\alpha)^{\frac{1}{2}} + 9b y^2 \big\} \\
& \quad - 135(1+b)^5 y y_0^4 + 36(1+b)^5 y_0^5 \Big]
\end{aligned}$$

+

$$
\begin{aligned}
&+\frac{3}{2240}\,a^5\Big[\,(14+259\,k^2+315\,k^4-7\,k^6-5\,k^8)\,y^{\frac{15}{2}}(y+\alpha)^{-\frac{1}{2}}\\
&\qquad+(93\,k+385\,k^3+119\,k^5-21\,k^7)\,y^7\\
&-63(1+k)^3y_0^2\Big\{(4+20\,k^2)\,y^5+(15\,k+10\,k^3-k^5)\,y^{\frac{11}{2}}(y+\alpha)^{-\frac{1}{2}}\Big\}\\
&+28(1+k)^3y_0^3\Big\{(25+140\,k^2+15k^4)\,y^4+(90\,k+70\,k^3-4k^5)\,y^{\frac{7}{2}}(y+\alpha)^{\frac{1}{2}}\Big\}\\
&-315(1+k)^5y_0^4\Big\{(2-k+4k^2+k^3)\,y^{\frac{7}{2}}(y+\alpha)^{-\frac{1}{2}}+6k\,y^3\Big\}\\
&-84(1+k)^5y_0^5\Big\{(1+10k-29k^2-20k^3)\,y^{\frac{3}{2}}(y+\alpha)^{\frac{1}{2}}-18k\,y^2\Big\}\\
&+35(1+k)^6y_0^6\Big\{(-8+24k^2)\,y^{\frac{1}{2}}(y+\alpha)^{\frac{1}{2}}+(-9k-57k^2)\,y\\
&\qquad+(48-48k^2)\,y\,L\Big\}\\
&+18(1+k)^7(14-11k)\,y_0^7\,\Big]\\
&+\frac{1}{537600}\,a^6\Big[\,5(280+8079\,k^2+19404\,k^4+7266\,k^6+2916\,k^8+711\,k^{10})\,y^9\\
&+5(2286\,k+16041\,k^3+14616\,k^5+3654k^7+1954k^9+1056k^{11})\,y^{\frac{9}{2}}(y+\alpha)^{-\frac{1}{2}}\\
&-540(1+k)^3y_0^2\Big\{(70+777\,k^2+315\,k^4+7k^6+15k^8)\,y^{\frac{17}{2}}(y+\alpha)^{-\frac{1}{2}}\\
&\qquad+(372\,k+770\,k^3+42\,k^5)\,y^7\Big\}\\
&+144(1+k)^3y_0^3\Big\{(889+11116\,k^2+6405k^4-770\,k^6+40\,k^8)\,y^{\frac{13}{2}}(y+\alpha)^{-\frac{1}{2}}\\
&\qquad+(4725\,k+11410\,k^3+189k^5-84k^7)\,y^6\Big\}\\
&-17010(1+k)^5y_0^4\Big\{(4-8\,k+60\,k^2)\,y^5\\
&\qquad+(30\,k-15k^2+40\,k^3+10k^4-6k^5-3k^6)\,y^{\frac{13}{2}}(y+\alpha)^{-\frac{1}{2}}\Big\}\\
&-7560(1+k)^5y_0^5\Big\{(70+100\,k-168k^2-78k^4-6k^5)\,y^4\\
&\qquad+(123\,k+240k^2-242k^3-140k^4+15k^5+12k^6)\,y^{\frac{9}{2}}(y+\alpha)^{-\frac{1}{2}}\Big\}\\
&+1260(1+k)^6y_0^6\Big\{(220+450\,k^2-1710\,k^3+660\,k^4)\,y^3\\
&\qquad+(450+540\,k-855k^2-685k^3-165k^4-37k^5)\,y^{\frac{5}{2}}(y+\alpha)^{-\frac{1}{2}}\\
&\qquad+[(720-720\,k^4)\,y^{\frac{5}{2}}(y+\alpha)^{\frac{1}{2}}+(1440\,k-1440k^3)\,y^3]\,L\Big\}\\
&-3240(1+k)^7y_0^7\Big\{(490+785\,k-672k^2-797k^3-280k^4)\,y^{\frac{5}{2}}(y+\alpha)^{-\frac{1}{2}}+(-252\,k+198k^2)\,y^2\Big\}\\
&+567(1+k)^8y_0^8\Big\{(2272+1090\,k-8107k^2-5005k^3)\,y+(-1280-800\,k+5440k^2\\
&\qquad+4000k^3)\,y^{\frac{1}{2}}(y+\alpha)^{\frac{1}{2}}+(320+320\,k)(11-6k-15k^2)\,y\,L\Big\}\\
&+40(1+k)^9y_0^9\Big\{(8386-2286\,k-23097k^2)+(5040-15120k^2)\,L\Big\}\,\Big]\\
&+\ldots\\
&\text{where}\quad L=\operatorname{aresinh}(y/\alpha)^{\frac{1}{2}}-\ln(4y_0/\alpha)^{\frac{1}{2}}\,. \qquad (8.2.1)
\end{aligned}
$$

Now this is substituted one more time into (8.1. 4/5), setting $y = 0$ there; with

$$\Lambda = \ln(\alpha/4y_0) = \ln\left[\tfrac{1}{4}\, a\,(1+k)^3 y_0^2\right] \qquad (8.2.\ 2)$$

we obtain

$$\begin{aligned}
\varphi(0) = {} & a^3 (1+k)^3 y_0^3 \\
& + \tfrac{9}{20}\, a^4 (1+k)^5 y_0^5 + \tfrac{27}{1120}\, a^5 (1+k)^7 y_0^7 (14 - 11k) \\
& + \tfrac{1}{13\,440}\, a^6 (1+k)^9 y_0^9 \left[8386 - 2286k + 2309 7k^2 \right. \\
& \qquad \left. + (2520 - 7560k^2)\,\Lambda \right] \\
& + \tfrac{3}{3942\,400}\, a^7 (1+k)^{11} y_0^{11} \left[2298\,856 + 963730k - 10\,531\,022k^2 \right. \\
& \qquad - 6874\,325k^3 \\
& \qquad \left. + 110\,880\,(8 + 5k + 16k^2 + 25k^3)\,\Lambda \right] \\
& + \ldots \qquad , \qquad (8.2.\ 3)
\end{aligned}$$

and

$$\begin{aligned}
\varphi'(0) = {} & a^2 - \tfrac{3}{2}\, a^3 (1+k)^3 y_0^2 - \tfrac{27}{16}\, a^4 (1+k)^5 y_0^4 \\
& + \tfrac{9}{64}\, a^5 (1+k)^6 y_0^6 \left[-3k - 19k^2 + (8 - 8k^2)\,\Lambda \right] \\
& + \tfrac{27}{25600}\, a^6 (1+k)^9 y_0^8 \left[2272 + 1090k - 8107k^2 - 5005k^3 \right. \\
& \qquad \left. + 160\,(1+k)(11 - 6k - 15k^2)\,\Lambda \right] \\
& + \tfrac{81}{2508\,800}\, a^7 (1+k)^{10} y_0^{10} \left[2273\,488 + 1627\,070k - 803 9\,458k^2 \right. \\
& \qquad - 9415\,165k^3 - 2862\,125k^4 \\
& \qquad \left. + 1680\,(1+k)(672 - 117k - 870k^2 - 875k^3)\,\Lambda \right] \\
& + \ldots \qquad . \qquad (8.2.\ 4)
\end{aligned}$$

Substituting φ in terms of a into (1.3. 10/11) yields for pressure and energy the expressions

$$p v = \frac{2 \cdot 3^{\frac{1}{3}}}{15} \frac{Z^2 e^2}{\mu} a^5 (1+k)^4 y_0^3 \left(1 - \tfrac{1}{4} k\right) , \qquad (8.2.\ 5)$$

and

$$\int_0^{y_0} z^{-\frac{1}{2}} \left[\varphi^{\frac{1}{2}} + \beta z^{\frac{1}{2}}\right]^3 \left[\varphi - 3\beta z^{\frac{1}{2}} \varphi^{\frac{1}{2}} - 9\beta^2 z\right] dz =$$

$$= \tfrac{1}{3} a^5 (1+k)^3 y_0^3 (1 - 3k - 9k^2) + \tfrac{1}{4} a^6 (1+k)^5 y_0^5 (1 - 2k - 6k^2)$$

$$+ \frac{9}{224} a^7 (1+k)^7 y_0^7 (12 - 13k - 28k^2 + 22k^3)$$

$$+ \tfrac{1}{8064} a^8 (1+k)^9 y_0^9 \left[1232 - 2340k - 22\,869k^2 + 4572k^3 + 46\,194k^4 - 2520(1 + 3k^2 - 6k^4)\Lambda\right]$$

$$+ \frac{1}{2365\,440} a^9 (1+k)^{11} y_0^{11} \left[-1\,486\,912 - 1\,343\,290k - 20\,109\,312k^2 - 9269\,145k^3 + 63\,186\,132k^4 + 41\,245\,950k^5 - 110\,880(14 + 5k + 72k^2 + 45k^3 + 96k^4 + 150k^5)\Lambda\right]$$

$$+ \ldots . \qquad (8.2.\ 6)$$

We want to remark here that the evaluation of the integral (8.2. 6) represents the real success of our method: only thanks to the approximation (8.2. 1) to $\varphi(y)$ is it possible to perform this integration explicitly. Thus, for the first time, the energy can be explicitly expressed as a function of the boundary radius and of the exchange parameter β_0 .

According to (8.1. 2) $\varphi(0) = 1$ is now substituted into (8.2. 3). The resultant series is easily reverted to give a as a series in y_0 ; this can be substituted into (8.2. 4-6) to yield pv and E (1.3. 10/11). Analogous to section 7.2 we check our expansion by means of the relation

$$p v = -\tfrac{1}{3} y_0 \frac{\partial E}{\partial y_0} . \qquad (8.2.\ 7)$$

Before actually writing down the expansion for a we want to note that not only can it be verified by means of (8.2. 7) but in addition one more term in the expansion can be obtained from (8.2. 7) with relative ease. For obviously (8.2. 4) for $\varphi'(0)$ and (8.2. 5) for ρ_v have already been evaluated to fifth order: since according to (8.1. 7) $b = O(y_0)$ we need in (8.2. 6) only the pure TF term which can be evaluated from (1.2.14). Thus having at our disposal all the fifth-order terms we write the expected form of the fifth-order term in a with undetermined numerical coefficients and substitute this into (8.2. 7). By equating coefficients of corresponding powers on both sides of the resulting expression the correct coefficients are then obtained.

Including the term obtained by the procedure just described finally leads to

$$
\begin{aligned}
a = y_0^{-1}\Big[\, 1 &- \tfrac{1}{20}\, y_0 \{3 + 20\beta\} - \tfrac{3}{200}\, y_0^2 \{3 + 10\beta\} \\
&- \frac{1}{100\,800}\, y_0^3 \{7(1861 + 900 \ln \tfrac{y_0}{4}) + 2430\,\beta + 15\,120\,\beta^2\} \\
&- \frac{1}{36\,960\,000}\, y_0^4 \{7\,(1895\,071 + 792000 \ln \tfrac{y_0}{4}) + 880\,\beta\,(23\,486 + 7875 \ln \tfrac{y_0}{4}) \\
&\qquad - 2316\,600\,\beta^2 + 5544\,000\,\beta^3\} \\
&- \frac{1}{9609\,600\,000}\, y_0^5 \{792\,(12\,964\,591 + 5\,118\,750 \ln \tfrac{y_0}{4}) \\
&\qquad + 325\,\beta\,(63\,409\,807 + 23\,007\,600 \ln \tfrac{y_0}{4}) \\
&\qquad + 143000\,\beta^2\,(52397 + 12\,600 \ln \tfrac{y_0}{4}) \\
&\qquad - 2069\,496\,000\,\beta^3 + 1441\,440\,000\,\beta^4\} \\
&+ \ldots\ldots \Big]
\end{aligned}
\qquad (8.2.\ 8)
$$

The corresponding expansions for $\varphi^0 = \varphi(y_0) = a^2 y_0$ and $\varphi'(0) = 3^{\frac{2}{3}} B$ then follow immediately. Thus we have achieved our aim: to find the boundary values of φ as functions of $x_0 = 3^{\frac{1}{3}} y_0$. These expansions, which are of the same type as (8.2. 8), will not be written explicitly.

In the next section expansions for the equation of state and the energy will be derived from the results obtained above, and compared with similar expansions derived in many-body theory.

8.3 . Expansions for pressure and energy

In the previous section we found expressions for $p v$, $[d\varphi/dy]_{y=0}$ and the integral in (1.3.10), involving the parameter a, and also an expansion for this parameter in powers of the boundary radius y_0 and its logarithm. It is quite easy to derive from this expansions for pressure and energy as functions of the atomic volume. It is simplest to express all quantities in y_0 and β; we remember that these are connected to the atomic volume v and the atom number Z by

$$y_0 = \frac{8\pi}{3}\,\frac{me^2}{h^2}\,(4Zv)^{\frac{1}{3}} \quad ; \quad \beta = \tfrac{1}{2}\left(\frac{3}{2\pi Z}\right)^{\frac{2}{3}} . \qquad (8.3.1)$$

For the pressure one has

$$p = \frac{2}{3} c_k \left(\frac{Z}{v}\right)^{\frac{5}{3}} \Big[\, 1 - \tfrac{1}{4} y_0 (3+5\beta)$$
$$- \frac{1}{100\,800} y_0^3 \{ 7(7847 + 4500 \ln \tfrac{y_0}{4}) - 38880\,\beta \}$$
$$- \frac{1}{2217\,600} y_0^4 \{ 63(49789 + 19800 \ln \tfrac{y_0}{4}) + 220\beta(21451 + 6300 \ln \tfrac{y_0}{4}) - 1710\,720\,\beta^2 \}$$
$$- \frac{3}{3203\,200\,000} y_0^5 \{ 3(1510\,087\,837 + 585\,585\,000 \ln \tfrac{y_0}{4}) + 1950\beta(3942\,109 + 1386\,000 \ln \tfrac{y_0}{4}) + 1484\,912\,000\,\beta^2 - 1235\,520\,000\,\beta^3 \} + \ldots \Big] , \qquad (8.3.2)$$

and for the energy

$$E = c_k Z^{\frac{2}{3}} v^{-\frac{2}{3}} \Big[\, 1 - \tfrac{1}{2} y_0 (3+5\beta) - \frac{27}{35} y_0^2$$
$$+ \frac{1}{50400} y_0^3 \{ 7(3347 + 4500 \ln \tfrac{y_0}{4}) - 38880\,\beta \}$$
$$+ \frac{1}{2217600} y_0^4 \{ 63(39889 + 19800 \ln \tfrac{y_0}{4}) + 220\beta(18301 + 6300 \ln \tfrac{y_0}{4}) - 1710\,720\,\beta^2 \}$$
$$+ \frac{1}{160\,600\,000} y_0^5 \{ 3(1314\,892\,837 + 585\,585\,000 \ln \tfrac{y_0}{4}) + 1950\beta(3480\,109 + 1386\,000 \ln \tfrac{y_0}{4}) + 1484\,912\,000\,\beta^2 - 1235\,520\,000\,\beta^3 \}$$
$$+ \ldots \Big] . \qquad (8.3.3)$$

The leading terms in these expansions are obviously the pressure and energy of a degenerate free electron gas of density (Z/v). This is the average electron density over the atom; as the atomic volume, and thus y_0, decreases, the point character of the nuclear charge becomes irrelevant and its effect approaches that of the uniform background of the free-electron model.

It is instructive to compare (8.3. 3) with expansions for the correlation energy of a free electron gas obtained by modern many-body methods. For this purpose we consider the expansion due to Gell-Mann and Brueckner [3]. In the usual many-body notation, we express the energy per electron $\varepsilon = E/Z$ in Rydberg units, and the volume per electron v/Z in a dimensionless parameter r_s such that $v/Z = \frac{4}{3}\pi a_0^3 r_s^3$ or

$$y_0 = 2 r_s \left(\frac{4Z}{9\pi}\right)^{\frac{2}{3}} \qquad (8.3.\ 4)$$

For the first few terms we find, substituting numerical values in (8.3. 3):

$$\varepsilon = \frac{2.21}{r_s^2} - \frac{0.916 + 1.8 Z^{\frac{2}{3}}}{r_s} - 0.503\, Z^{\frac{4}{3}}$$

$$- r_s \left[0.0834\, Z^{\frac{4}{3}} + \left(0.277 - 0.221 \ln Z^{\frac{2}{3}} r_s\right) Z^2\right] + \cdots \qquad (8.3.\ 5)$$

while the GB series, in the same units, is

$$\varepsilon = \frac{2.21}{r_s^2} - \frac{0.916}{r_s} - \left[0.096 - 0.0622 \ln r_s\right] + \cdots \qquad (8.3.\ 6)$$

Naturally enough the leading terms, representing the free-electron energy, are equal. The first-order correction contains the exchange energy in both expansions, but in ours, in addition, a numerically much larger contribution. In second order we obtain a constant against the logarithmic term of GB; ours is much larger in magnitude unless r_s would be less than the radius of the electron. Our first logarithmic term appears in third order.

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3) M. Gell-Mann & K.A. Brueckner, Phys.Rev. 106 (1957) 364-8, referred to as GB.

This completes our treatment of the TF and TFD atoms. We have seen that the solution is essentially different according to the magnitude of the boundary radius; for small x_0 logarithmic terms appear, and special care has to be taken in order to obtain the correct expansions.

CHAPTER 9 . PROBLEMS IN OTHER FIELDS OF PHYSICS TO WHICH SIMILAR METHODS COULD BE APPLIED

The methods developed in this thesis, which proved successful in treating the Thomas-Fermi equation to a degree of accuracy far beyond original expectations, could we feel profitably be applied in several other fields of physics. This will be illustrated by briefly discussing (i) some differential equations of a similar nature or involving two-point boundary conditions, and (ii) problems where it is necessary to analyse power series in order to determine location and nature of the singularities of the corresponding functions. We hope to show that application of some of our methods can lead to improvements here.

9.1 . Differential equations

9.11. A class of equations closely related to the TF equation

First we will study a class of equations [1] of which the TF equation is a special case:

$$\frac{d^2y}{dx^2} = x^{-\frac{n}{n+1}}\, y^{\frac{2n+1}{n+1}} \quad . \tag{9.11.1}$$

This equation, which for $n=1$ reduces to the TF equation, can be analysed in exactly the same way as given in chapters 4, 5 and 6. For small x , we write

$$y = \sum_{\ell,s=0}^{\infty} a_{\ell,s}\, \left(x^{\frac{n+2}{n+1}}\right)^{\ell} (xB)^{s} \quad , \tag{9.11.2}$$

which then leads to either

$$y = \sum_{k=0}^{\infty} a_k \left(x^{\frac{1}{n+1}}\right)^{k} \quad , \quad a_k = a_k(B) \, ,$$

or

$$y = \sum_{s=0}^{\infty} b_s B^{s} \quad , \quad b_s = b_s(x) \, , \text{ as in chapter 4.}$$

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1) E. Kamke, Differentialgleichungen, Bd 1,6.Auflage, Leipzig (1959), equation (C6.102),p.569, where further references are given.

For large x, there is a particular solution analogous to the Sommerfeld solution:

$$y_0(x) = \left[2\frac{(n+1)(n+2)}{n^2}\right]^{\frac{n+1}{n}} x^{-\frac{n+2}{n}} \quad ; \qquad (9.11.3)$$

one can again write $y = y_0 \psi$ and find

$$\frac{n^2}{(n+1)(n+2)} x^2 \psi'' - \frac{2n}{n+1} x\psi' + 2\psi = 2\psi^{\frac{2n+1}{n+1}} \quad . \qquad (9.11.4)$$

Like (5.1. 4), this equation has series solutions in $x = Fx^\lambda$ with

$\lambda = \lambda_\pm = \frac{3n+4 \pm \sqrt{17n^2+40n+16}}{2n}$. Retaining only λ_-, we obtain an equation analogous to (5.1. 9), which here too has a nearly exact solution, of the form $(1+\beta x)^{-2\frac{n+1}{n}}$; the analysis proceeds along the same lines as in chapter 5. Retaining both roots λ_- and λ_+, we arrive at the analogon of (6.1. 7), and we can make transformations as in chapter 6.

9.12. The Emden equation

As a second example, we consider the equation

$$x\frac{d^2y}{dx^2} + 2\frac{dy}{dx} + xy^n = 0 \qquad (9.21.1)$$

This is Emden's differential equation [2,3]: it describes a polytropic sphere of gas of index $\frac{n+1}{n}$ in gravitational equilibrium. Here x is a dimensionless radial variable and y^n is proportional to the density. Writing $y = x^{-1}\varphi$ leads to

$$\frac{d^2\varphi}{dx^2} + x^{1-n}\varphi^n = 0 \quad ; \qquad (9.12.2)$$

in this form one recognizes the similarity between the Emden and

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2) R. Emden, Gaskugeln, B.G. Teubner, Berlin-Leipzig, 1907; see also E. Kamke, ref.[1], equation (C6.74), p. 560-1.

3) E.A. Milne, Montly Notices Roy.Astr.Soc. 91 (1931) 4-55; R.H. Fowler, ibid., 63-91.

TF equations, apart from the sign of the second term in (9.12.2). Thus it is expected that similar methods may be applicable here too. Milne [3] finds that (9.12.1) with $n = 3$ and $y \propto T$ describes the equilibrium of a sphere of perfect gas of constant opacity, containing a uniform distribution of radiant energy sources. A similar sphere, but then of degenerate gas, is described by the same equation with $n = \frac{3}{2}$ and $y^{\frac{3}{2}}$ proportional to the density.

9.13. The Prandtl-Blasius boundary layer equation

As a last example we treat a non-linear two-point boundary-value problem to which our method of joining different expansions could possibly be applied: the Prandtl-Blasius equation of boundary layer theory. The equation describes [4] the stream function in the boundary layer of viscous flow past a flat plate at high Reynolds number. With the independent variable η connected to the perpendicular distance from the plate, and the function $f(\eta)$ connected with the stream function, the equation has the form

$$f''' + f f'' = 0 \qquad (9.13.1)$$

with the boundary conditions

$$f(0) = f'(0) = 0 \quad , \quad f'(\infty) = 1 \quad . \qquad (9.13.2)$$

We expect that our technique of expanding f for small and for large η and matching the expansions at an intermediate point should be applicable here too. For small η, it is easily shown that

$$f(\eta) = A\eta^2 \varphi(A\eta^3) \qquad (9.13.3)$$

where A is a parameter and

$$\varphi(z) = 1 - \tfrac{1}{30} z + \tfrac{11}{5040} z^2 - \tfrac{5}{33264} z^3 + \ldots \quad . \qquad (9.13.4)$$

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4) E.g. H. Schlichting, Boundary Layer Theory, 4th Ed., Mc.Graw Hill (1960) 116-20; M. Van Dyke, Perturbation Methods in Fluid Mechanics, Academic Press (1964) 129-32.

For large η one has

$$f(\eta) = \eta - \beta + \gamma \int^{\eta} d\eta' \int^{\eta'} d\eta'' \, e^{-\frac{1}{2}(\eta''-\beta)^2} + \ldots \,, \quad (9.13.5)$$

with β and γ parameters. These expansions would have to be extended to cover the whole range $0 \leq \eta \leq \infty$; admittedly this is much more difficult than in our case, specially for (9.13.5).

9.2 . Analysis of series expansions

The main impetus in this field came from the work on critical phenomena [5], including such subjects as the behaviour of vapour near the critical point, of a ferromagnet near the Curie point or an antiferromagnet near its Néel point, of a superfluid near the transition temperature and of an alloy near the ordering temperature. To account for these phenomena, Ising-type models are commonly adopted, while in magnetic theory the Heisenberg model is treated very often as well. In these models, quantities like magnetization, or in general any quantity describing a low-temperature ordering, and magnetic susceptibility or specific heat, can be expressed as power series in the temperature or its inverse, according as the temperature is low or high. At the cost of hard labour it is possible to calculate a limited number of coefficients in such expansions, typically 9 or 10 (see Domb [6] for a survey of methods). All information on the critical temperature, etc. must be extracted from these series.

In the following we will not discuss a special case, nor try to convey the exact physical meaning of the variables. Instead we will consider the more abstract mathematical problem involved throughout, which can be stated as follows: suppose one has available a limited number of terms of the series

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5) For recent review articles, see L.P. Kadanoff et.al., Rev.Mod. Phys. 39 (1967) 395-431; M.E. Fisher, Rep.Prog.Phys. 30 (1967) 615-730 (theory); P. Heller, Rep.Prog.Phys. 30 (1967) 731-826 (experiment).

6) C. Domb, Adv.Phys. 9 (1960) 149-361.

$$f(x) = \sum_{n=0}^{\infty} a_n x^n \quad ; \tag{9.2. 1}$$

suppose also that one suspects that $f(x)$ has a singularity at x_e of the form

$$f(x) \approx A(1 - \frac{x}{x_e})^{-g} \quad , \quad x \approx x_e \quad . \tag{9.2. 2}$$

Our task is now to find, from the available a_n, x_e and g as accurately as possible. We present a short survey of methods commonly applied in this field, and compare these to our methods as developed in this thesis.

9.21. The "ratio" method of Domb and Sykes

Domb and Sykes [7] make, on physical grounds, the assumption that the coefficients a_n should behave for large n like

$$a_n \propto x_e^{-n} \, n^{g-1} \tag{9.21.1}$$

where x_e is a critical value. In that case, the ratio of successive coefficients would be

$$u_n \equiv \frac{a_n}{a_{n-1}} \approx x_e^{-1} \left[1 + \frac{g-1}{n}\right] \quad , \tag{9.21.2}$$

and we note that this relation would be exactly satisfied if $f(x)$ is of the form (9.2. 2). One way to obtain x_e and g from u_n is to plot u_n vs. n^{-1} : the slope of this curve, which ideally should be a straight line, gives g , while the intersection with $n^{-1} = 0$ yields the value of x_e . A second method is to form the "linear extrapolants"

$$u_n^{(i)} = \frac{1}{i}\left[n\, u_n^{(i-1)} - (n-i)\, u_{n-1}^{(i-1)}\right] \quad , \quad u_n^{(0)} = u_n \; ; \tag{9.21.3}$$

if (9.2. 2) holds exactly, then $u_n^{(i)} = x_e^{-1}$ for all $i \geq 1$; otherwise successive $u_n^{(i)}$ will, one hopes, tend to x_e^{-1} as a limit.

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7) C. Domb & M.F. Sykes, Proc.Roy.Soc.A 240 (1957) 214-28, and J.Mathematical Phys. 2 (1961) 63-7.

If one of the quantities x_e or q is known already, one can find the other as follows: if x_e is known, then one forms

$$g_n = n\,(u_n x_e - 1) + 1 \quad ; \tag{9.21.4}$$

ideally, $g_n \equiv q$; otherwise $\lim_{n\to\infty} g_n = q$. If q is known, one forms

$$\beta_n = \frac{n}{n+q-1}\, u_n \quad ; \tag{9.21.5}$$

ideally $\beta_n \equiv x_e^{-1}$, otherwise $\lim_{n\to\infty} \beta_n = x_e^{-1}$.

9.22. The Padé approximant method

With the help of the Padé approximants [8] (PA's) to the expansion (9.2. 1) (see also section 4.6) one tries to locate the singularity of $f(x)$ as the limit to which poles of successive PA's tend. As in the previous section, there are approaches applicable when both x_e and q are unknown and special methods if one of them is known already. In the first case we have two common methods:

(i) Form the expansion of $F_1(x) = d\,[\ln f(x)]/dx$ (9.22.1)

Ideally, $F_1 = \frac{q}{x_e - x}$; thus PA's to the expansion should have denominators with one simple root. In practice the roots of the denominators of successive approximants give an estimate of x_e, while the residues there yield values for q .

(ii) Form the expansion of

$$F_2(x) = \frac{f(x)\, f''(x)}{[f'(x)]^2} \quad . \tag{9.22.2}$$

If (9.2.2) holds near x_e , we should have there $F_2 \equiv \frac{q+1}{q}$; forming PA's to F_2 and evaluating these at trial values x_e should yield estimates for q which are rather insensitive to the choice of x_e .

In the second case , when x_e is known we can form

$$F_3(x) = (x_e - x)\,\frac{d}{dx} \ln f(x) \quad . \tag{9.22.3}$$

In the ideal case, $F_3(x) \equiv q$; evaluating PA's to the expansion of F_3 at x_e one obtains estimates for q . When q is known, one

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8) For a review, see G.A. Baker Jr., Adv.in Theor.Phys. 1 (1965) 1-58; see also G.A. Baker Jr., H.E. Gilbert, J. Eve & G.S. Rushbrooke, Phys.Rev. 164 (1967) nr.2, 800-17.

forms $$F_4(x) = [f(x)]^{\frac{1}{q}} \quad ; \qquad (9.22.4)$$

approximants to F_4 must have simple poles at values approaching x_e, since ideally $F_4 = A^{\frac{1}{q}}(1 - x/x_e)^{-1}$ by (9.2.2); the residues give the proportionality constant A.

9.23. Various other methods

(i) Starting from the assumption that $f(x)$ behaves like (9.2.2), Ninham and Thompson [9] evaluate the integral $\int_0^{x_e} f'(x)\,dx$ by means of a generalized Euler-MacLaurin summation formula with an asymptotic expansion for the remainder. The numerical value, obtained with trial values for x_e and q, is equal to $-f(0)$ if $q < 1$ and the integral converges; if $q \geq 1$ the numerical value is interpreted as the Hadamard finite part of the integral, which again is $-f(0)$. The difference between the value of the integral - as evaluated with the trial values - and $-a_0$ yields reliable estimates for the error in the values x_e and q adopted.

(ii) Guttmann, Ninham and Thompson [10] suppose that $f(x)$ can be written in the form

$$f(x) = (1 - \frac{x}{x_e})^{-q} h(x) \qquad (9.23.1)$$

Under certain conditions on the behaviour of $h(x)$ they show that the set of functions

$$h_n(x) = (1 + \frac{x}{x_e})^n \left[(1 - \frac{x}{x_e})^q f(x)\right] \qquad (9.23.2)$$

will have expansion coefficients $a_m^{(n)}$ which for large m oscillate in sign and decrease in magnitude, if x_e and q in (9.23.2) correspond to the actual singularity of $f(x)$. Thus for $n = 0, 1, 2, \ldots$ one can find a region in the $x_e - q$ plane where the $a_m^{(n)}$ indeed show this behaviour. This yields values for x_e and q, together with error estimates; these become narrower as n is increased.

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9) B.W. Ninham & C.J. Thompson, (unpublished); B.W. Ninham, Numerische Math. 8 (1966) 444-57; J.N. Lyness & B.W. Ninham, Math.Comp. 21 (1967) 162-78.

10) A.J. Guttmann, B.W. Ninham & C.J. Thompson, Phys.Letters 26 A (1968) nr.5, 29 Jan., 180-1.

9.24. Comparison with the methods applied in this work

This chapter will be concluded with a brief comparison between the methods developed in this thesis and those discussed above.

As regards the ratio method: the technique described by equations (4.2.7-9) bears a close resemblance to this method. Nevertheless we feel that our method of extrapolating might be slightly better; also better estimates for x_c are obtained if instead of (9.2. 2) the coefficients a_n are fitted to a hypergeometric series. The introduction of the Darboux form (4.2. 4) again enables us to refine the estimates considerably.

By comparing with section 9.22, we see that in the PA method x_c is normally determined as the zero of the denominator of successive PA's. However, in the calculation of these approximants the early coefficients have a relatively large influence, and may obscure the behaviour exhibited by the late coefficients. Therefore, where $q<0$ as in our sections 4.3, 4.5 and 6.31, it is preferable to find x_c directly from the series instead of via the PA's. Naturally this depends on the behaviour of the contributions to $f(x)$ which are non-singular near x_c ; we were fortunate in that these vanished at x_c as well. For $q>0$, it seems to us that it should be equally possible to find x_c as the zero of $[f(x)]^{-\frac{1}{q}}$ instead of applying (9.22.4) and its PA's, especially if convergence-improving techniques (appendix 10.2) are judiciously applied. Of course, if a differential equation for $f(x)$ is available, this can yield a large amount of additional information, as demonstrated by the analysis of section 4.3 .

Finally, we consider the improvements which can be achieved once x_c and q , and also A of (9.2. 2) are known. Most commonly applied is the method of subtracting one contribution as in (4.4.17); we feel that, where possible, the subtraction of more Darboux-type terms could increase the accuracy of the resulting series considerably. When a contribution of the type discussed above is dominant, the method of (4.4.18), dividing out this contribution, yields very great improvement. On the other hand,

truncation effects make it necessary to employ x_c -values known to many decimals, and it is very difficult to obtain these from series analysis alone. In effect, it was only our application of the differential equations to find the exact value of q and a very accurate estimate of x_c that enabled us to introduce this method. In most of the Ising-like models one is not so fortunate as to have such auxiliary knowledge of the function $f(x)$ concerned.

CHAPTER 10. APPENDICES

In this chapter we have brought together some numerical or mathematical considerations which if discussed in the main body of the thesis/ would have made it needlessly hard to digest.

10.1 . Tabulation of some solutions to the TF equation

In this first section we calculate several solutions to the TF equation, obtaining numerical values by means of the power series expansions derived earlier in this thesis. Tables are given of the solution for the isolated atom, and of March's Master Solutions.

10.11. The TF function for the isolated atom

For the isolated atom, the TF function is described by the Baker series with $B = -1.5880710226$ and by the CM series with $F = 13.270973848$. To calculate φ and φ' for $0 \leq x \leq 1$, the Padé approximants (4.6. 3) to the Baker series are employed. In order to avoid difficulties caused by the singularity at the origin, the function is tabulated at equal intervals in $x^{\frac{1}{2}}$. For $1 < x < \infty$ we apply the modification of the CM series given by (5.4. 3/5); here the tabulation is in equal increments of x.

The tabular intervals are chosen in such a way that full tabular accuracy can be reached by 4- or 5-point Lagrangian interpolation [1] for φ and φ' respectively. Thus, for $0 \leq x \leq 1$, we have

$$\varphi\left(\left[x_0^{\frac{1}{2}} + ph\right]^2\right) = \sum_{k=-1}^{2} A_k^4(p)\, \varphi(x_k) \quad , \qquad (10.11.1)$$

where $A_k^n(p)$ are n-point Lagrangian interpolation coefficients [1] and $x_k^{\frac{1}{2}} = x_0^{\frac{1}{2}} + kh$. A similar expression, with 5-point interpolation, holds for φ' . For $x > 1$, since here φ behaves almost

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1) See e.g. Handbook of Mathematical Functions, National Bureau of Standards, Applied Mathematics Series 55, 3rd Ed. (1965) Section 25.2 and table 25.1.

like x^{-3} and φ' almost like x^{-4}, it is advantageous to perform the interpolation on the inverse of φ or φ':

$$\varphi^{-1}(x_0 + ph) = \sum_{k=-1}^{2} A_k^4(p)\, \varphi^{-1}(x_k) \quad , \qquad (10.11.2)$$

and similarly for φ' with a 5-point formula.

The function values thus calculated are listed in table 10.1. They agree with those of Kobayashi et.al. [2] to the accuracy given by those authors.

10.12. The "Master Solutions" of March

March [3] has calculated by a numerical-integration method two typical solutions to the TF equation; these are of the CM type and are defined by putting $F_- \pm 1$ in (5.1. 7). Any solution with an arbitrary value of F can be found from one of these by the scale transformation discussed in section 2.3. From the expansion (5.3. 1) for $\chi(z)$ these two solutions can be calculated quickly and accurately over a wide range of x.

As part of a research project in her final year of studies for an Honours Degree in Physics with Theoretical Physics, Miss Shona Wallace recalculated these Master Solutions to very high accuracy [4]. In tables 10.2 and 10.3 we present an extract from her tables. The intervals are once again chosen in such a manner that full tabular accuracy is achieved by 4- or 5-point Lagrangian interpolation, as in (10.11.2).

10.2. Convergence-improving techniques: Shanks' e_k -transforms

Often in the course of this work we have encountered the problem of numerically calculating the sum of a series for a value of the argument very near its radius of convergence. Here formally

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2) S. Kobayashi, T. Matsukuma, S. Nagai & K. Umeda, J.Phys.Soc.Japan 10 (1955) 759-62.

3) N.H. March, Proc.Camb.Phil.Soc. 48 (1952) 665-82.

4) S.H. Wallace, (unpublished).

The TF function $\varphi(x)$

x	$\varphi(x)$	$-\varphi'(x)$	x	$\varphi(x)$	$-\varphi'(x)$
0.0000	.10000000E+01	.15880710E+01	.1156	.86647761E-00	.95649783E-00
.0001	.99984253E-00	.15680726E+01	.1296	.85331290E-00	.92460076E-00
.0004	.99937544E-00	.15480836E+01	.1444	.83986238E-00	.89344141E-00
.0009	.99860672E-00	.15281131E+01	.1600	.82616492E-00	.86302859E-00
.0016	.99754436E-00	.15081701E+01	.1764	.81225747E-00	.83336864E-00
.0025	.99619630E-00	.14882632E+01	.1936	.79817511E-00	.80446559E-00
.0036	.99457047E-00	.14684008E+01	.2116	.78395104E-00	.77632134E-00
.0049	.99267476E-00	.14485912E+01	.2304	.76961664E-00	.74893579E-00
.0064	.99051702E-00	.14288421E+01	.2500	.75520147E-00	.72230698E-00
.0081	.98810506E-00	.14091613E+01	.2704	.74073334E-00	.69643129E-00
.0100	.98544661E-00	.13895561E+01	.2916	.72623834E-00	.67130352E-00
.0121	.98254938E-00	.13700337E+01	.3136	.71174089E-00	.64691707E-00
.0144	.97942100E-00	.13506008E+01	.3364	.69726379E-00	.62326402E-00
.0169	.97606901E-00	.13312642E+01	.3600	.68282826E-00	.60033535E-00
.0196	.97250090E-00	.13120301E+01	.4096	.65415931E-00	.55660981E-00
.0225	.96872410E-00	.12929047E+01	.4624	.62587454E-00	.51564926E-00
.0256	.96474590E-00	.12738938E+01	.5184	.59809291E-00	.47735106E-00
.0289	.96057357E-00	.12550030E+01	.5776	.57091367E-00	.44160405E-00
.0324	.95621425E-00	.12362377E+01	.6400	.54441817E-00	.40829120E-00
.0361	.95167500E-00	.12176029E+01	.7056	.51867163E-00	.37729186E-00
.0400	.94696277E-00	.11991035E+01	.7744	.49372484E-00	.34848368E-00
.0441	.94208444E-00	.11807440E+01	.8464	.46961581E-00	.32174421E-00
.0484	.93704676E-00	.11625290E+01	.9216	.44637126E-00	.29695228E-00
.0529	.93185639E-00	.11444625E+01	1.0000	.42400805E-00	.27398905E-00
.0576	.92651987E-00	.11265484E+01	1.0500	.41064548E-00	.26067456E-00
.0625	.92104365E-00	.11087905E+01	1.1000	.39792530E-00	.24827812E-00
.0676	.91543406E-00	.10911921E+01	1.1500	.38580379E-00	.23671447E-00
.0729	.90969731E-00	.10737566E+01	1.2000	.37424123E-00	.22590859E-00
.0784	.90383950E-00	.10564870E+01	1.2500	.36320141E-00	.21579413E-00
.0841	.89786663E-00	.10393862E+01	1.3000	.35265128E-00	.20631218E-00
.0900	.89178456E-00	.10224567E+01	1.3500	.34256053E-00	.19741026E-00
.1024	.87931573E-00	.98912120E-00	1.4000	.33290137E-00	.18904143E-00

Table 10.1

Table 10.1

(continued)

x	$\varphi(x)$	$-\varphi'(x)$	x	$\varphi(x)$	$-\varphi'(x)$
1.5000	.31477746E-00	.17373880E-00	7.0000	.46097819E-01	.11142532E-01
1.6000	.29809771E-00	.16011501E-00	7.5000	.40962466E-01	.94582646E-02
1.7000	.28270644E-00	.14793339E-00	8.0000	.36587255E-01	.80886030E-02
1.8000	.26846951E-00	.13699844E-00	8.5000	.32833089E-01	.69641638E-02
1.9000	.25527065E-00	.12714729E-00	9.0000	.29590935E-01	.60330747E-02
2.0000	.24300851E-00	.11824319E-00	9.5000	.26774390E-01	.52560300E-02
2.1000	.23159432E-00	.11017054E-00	10.0000	.24314293E-01	.46028819E-02
2.2000	.22094998E-00	.10283098E-00	11.0000	.20250365E-01	.35798152E-02
2.3000	.21100650E-00	.96140350E-01	12.0000	.17063922E-01	.28305364E-02
2.4000	.20170270E-00	.90026276E-01	13.0000	.14526518E-01	.22705246E-02
2.5000	.19298412E-00	.84426187E-01	14.0000	.12478406E-01	.18445014E-02
2.6000	.18480215E-00	.79285763E-01	15.0000	.10805359E-01	.15153231E-02
2.7000	.17711323E-00	.74557647E-01	16.0000	.94240789E-02	.12574353E-02
2.8000	.16987826E-00	.70200388E-01	17.0000	.82727639E-02	.10528868E-02
2.9000	.16306201E-00	.66177580E-01	18.0000	.73048459E-02	.88883111E-03
3.0000	.15663267E-00	.62457131E-01	19.0000	.64847464E-02	.75592142E-03
3.2000	.14482225E-00	.55813027E-01	20.0000	.57849412E-02	.64725433E-03
3.4000	.13424700E-00	.50077116E-01	21.0000	.51838934E-02	.55766158E-03
3.6000	.12474104E-00	.45097630E-01	22.0000	.46645758E-02	.48322574E-03
3.8000	.11616570E-00	.40752738E-01	23.0000	.42133981E-02	.42094370E-03
4.0000	.10840426E-00	.36943758E-01	24.0000	.38194181E-02	.36848922E-03
4.2000	.10135787E-00	.33590097E-01	25.0000	.34737544E-02	.32404300E-03
4.4000	.94942309E-01	.30625444E-01	26.0000	.31691444E-02	.28616952E-03
4.6000	.89085440E-01	.27994861E-01	27.0000	.28996077E-02	.25372672E-03
4.8000	.83725163E-01	.25652543E-01	28.0000	.26601879E-02	.22579901E-03
5.0000	.78807779E-01	.23560075E-01	29.0000	.24467526E-02	.20164709E-03
5.2000	.74286647E-01	.21685062E-01	30.0000	.22558366E-02	.18067001E-03
5.4000	.70121097E-01	.20000050E-01	32.0000	.19303255E-02	.14636106E-03
5.6000	.66275527E-01	.18481657E-01	34.0000	.16651908E-02	.11988459E-03
5.8000	.62718665E-01	.17109884E-01	36.0000	.14469544E-02	.99177175E-04
6.0000	.59422949E-01	.15867550E-01	38.0000	.12656139E-02	.82785536E-04
6.5000	.52172937E-01	.13235607E-01	40.0000	.11136356E-02	.69668029E-04

(continued)

Table 10.1

x	$\varphi(x)$	$-\varphi'(x)$	x	$\varphi(x)$	$-\varphi'(x)$
42.0000	.98526900E-03	.59066139E-04	220.0000	.11059515E-04	.14319926E-06
44.0000	.87607064E-03	.50419538E-04	230.0000	.97430901E-05	.12087522E-06
46.0000	.78256914E-03	.43308848E-04	240.0000	.86280670E-05	.10274431E-06
48.0000	.70202472E-03	.37416400E-04	250.0000	.76772908E-05	.87894680E-07
50.0000	.63225478E-03	.32498902E-04	260.0000	.68615484E-05	.75637915E-07
52.0000	.57150554E-03	.28368126E-04	270.0000	.61576544E-05	.65448528E-07
54.0000	.51835649E-03	.24877065E-04	280.0000	.55470471E-05	.56921313E-07
56.0000	.47164854E-03	.21909904E-04	290.0000	.50147464E-05	.49740861E-07
58.0000	.43042933E-03	.19374655E-04	300.0000	.45485720E-05	.43659496E-07
60.0000	.39391137E-03	.17197700E-04	320.0000	.37764638E-05	.34049389E-07
65.0000	.31914329E-03	.12960411E-04	340.0000	.31699637E-05	.26947014E-07
70.0000	.26226530E-03	.99565334E-05	360.0000	.26868955E-05	.21605808E-07
75.0000	.21821043E-03	.77779747E-05	380.0000	.22973543E-05	.17526291E-07
80.0000	.18354576E-03	.61661955E-05	400.0000	.19797326E-05	.14366823E-07
85.0000	.15588783E-03	.49526118E-05	420.0000	.17181518E-05	.11889056E-07
90.0000	.13354583E-03	.40244737E-05	440.0000	.15007645E-05	.99237154E-08
95.0000	.11529715E-03	.33046601E-05	460.0000	.13186086E-05	.83486285E-08
100.0000	.10024257E-03	.27393511E-05	480.0000	.11648192E-05	.70743170E-08
105.0000	.87710451E-04	.22903047E-05	500.0000	.10340772E-05	.60343634E-08
110.0000	.77192184E-04	.19299023E-05	520.0000	.92221765E-06	.51788589E-08
115.0000	.68297713E-04	.16379000E-05	540.0000	.82594795E-06	.44698733E-08
120.0000	.60724454E-04	.13992583E-05	560.0000	.74264155E-06	.38782777E-08
125.0000	.54235197E-04	.12026654E-05	580.0000	.67018590E-06	.33814850E-08
130.0000	.48642171E-04	.10395157E-05	600.0000	.60686877E-06	.29618225E-08
140.0000	.39574139E-04	.78856447E-06	650.0000	.47998446E-06	.21654695E-08
150.0000	.32633964E-04	.60913995E-06	700.0000	.38617652E-06	.16198322E-08
160.0000	.27231037E-04	.47807416E-06	750.0000	.31532580E-06	.12358341E-08
170.0000	.22961351E-04	.38051134E-06	800.0000	.26081373E-06	.95924386E-09
180.0000	.19542102E-04	.30666432E-06	850.0000	.21818665E-06	.75592724E-09
190.0000	.16771248E-04	.24992901E-06	900.0000	.18437242E-06	.60376618E-09
200.0000	.14501803E-04	.20575323E-06	950.0000	.15720504E-06	.48805717E-09
210.0000	.12625079E-04	.17093868E-06	1000.0000	.13512748E-06	.39880107E-09

Table 10.2

The master solution $\varphi_+(x)$ for $F = +1$

x	$\varphi_+(x)$	$-\varphi_+'(x)$	x	$\varphi_+(x)$	$-\varphi_+'(x)$
.12	.30808218E+04	.32637748E+05	.72	.12635491E+03	.39463125E+03
.13	.27775746E+04	.28157567E+05	.74	.11878543E+03	.36287915E+03
.14	.25150829E+04	.24455473E+05	.76	.11181862E+03	.33429742E+03
.15	.22864184E+04	.21368698E+05	.78	.10539492E+03	.30850984E+03
.16	.20860715E+04	.18774104E+05	.80	.99461772E+02	.28519172E+03
.17	.19096129E+04	.16577235E+05	.85	.86482589E+02	.23594469E+03
.18	.17534473E+04	.14704732E+05	.90	.75696366E+02	.19698635E+03
.19	.16146304E+04	.13098982E+05	.95	.66654418E+02	.16582248E+03
.20	.14907318E+04	.11714284E+05	1.00	.59014674E+02	.14064085E+03
.21	.13797307E+04	.10514044E+05	1.05	.52513085E+02	.12010514E+03
.22	.12799352E+04	.94687214E+04	1.10	.46943506E+02	.10321665E+03
.23	.11899204E+04	.85542796E+04	1.15	.42143324E+02	.89219783E+02
.24	.11084793E+04	.77510223E+04	1.20	.37983042E+02	.77536392E+02
.25	.10345838E+04	.70427027E+04	1.25	.34358630E+02	.67719516E+02
.26	.96735402E+03	.64158370E+04	1.30	.31185837E+02	.59420283E+02
.27	.90603330E+03	.58591701E+04	1.35	.28395918E+02	.52363957E+02
.28	.84996827E+03	.53632568E+04	1.40	.25932386E+02	.46332400E+02
.29	.79859234E+03	.49201310E+04	1.45	.23748526E+02	.41151070E+02
.30	.75141230E+03	.45230425E+04	1.50	.21805467E+02	.36679307E+02
.32	.66796953E+03	.38448294E+04	1.55	.20070683E+02	.32802989E+02
.34	.59678621E+03	.32918662E+04	1.60	.18516806E+02	.29428943E+02
.36	.53564296E+03	.28369140E+04	1.65	.17120700E+02	.26480641E+02
.38	.48279380E+03	.24594990E+04	1.70	.15862706E+02	.23894881E+02
.40	.43685077E+03	.21440360E+04	1.75	.14726049E+02	.21619185E+02
.42	.39669995E+03	.18785232E+04	1.80	.13696353E+02	.19609766E+02
.44	.36143955E+03	.16536204E+04	1.90	.11910054E+02	.16248702E+02
.46	.33033366E+03	.14619884E+04	2.00	.10423551E+02	.13581587E+02
.48	.30277726E+03	.12978081E+04	2.10	.91761780E+01	.11442691E+02
.50	.27826953E+03	.11564281E+04	2.20	.81214800E+01	.97108198E+01
.52	.25639327E+03	.10341012E+04	2.30	.72234663E+01	.82961167E+01
.54	.23679886E+03	.92778734E+03	2.40	.64539513E+01	.71311077E+01
.56	.21919168E+03	.83500383E+03	2.50	.57906432E+01	.61645364E+01
.58	.20332218E+03	.75371027E+03	2.60	.52157510E+01	.53570477E+01
.60	.18897797E+03	.68222006E+03	2.70	.47149555E+01	.46781239E+01
.62	.17597742E+03	.61913140E+03	2.80	.42766423E+01	.41038832E+01
.64	.16416455E+03	.56327312E+03	2.90	.38913220E+01	.36154764E+01
.66	.15340488E+03	.51366200E+03	3.00	.35511890E+01	.31979083E+01
.68	.14358198E+03	.46946880E+03	3.10	.32497822E+01	.28391606E+01
.70	.13459472E+03	.42999105E+03	3.20	.29817215E+01	.25295342E+01

Table 10.2

(continued)

x	$\varphi_+(x)$	$-\varphi_+'(x)$	x	$\varphi_+(x)$	$-\varphi_+'(x)$
3.30	.27425022E+01	.22611501E+01	9.40	.14576036E-00	.44487225E-01
3.40	.25283327E+01	.20275687E+01	9.60	.13721393E-00	.41035241E-01
3.50	.23360058E+01	.18234963E+01	9.80	.12932434E-00	.37912251E-01
3.60	.21627964E+01	.16445575E+01	10.00	.12202957E-00	.35081287E-01
3.70	.20063784E+01	.14871171E+01	10.50	.10604796E-00	.29080007E-01
3.80	.18647581E+01	.13481402E+01	11.00	.92744855E-01	.24310629E-01
3.90	.17362202E+01	.12250813E+01	11.50	.81581054E-01	.20481466E-01
4.00	.16192831E+01	.11157960E+01	12.00	.72142676E-01	.17378383E-01
4.10	.15126626E+01	.10184701E+01	12.50	.64108421E-01	.14842093E-01
4.20	.14152420E+01	.93156290E-00	13.00	.57226265E-01	.12752656E-01
4.30	.13260468E+01	.85376082E-00	13.50	.51296626E-01	.11018750E-01
4.40	.12442240E+01	.78393988E-00	14.00	.46160055E-01	.95701209E-02
4.50	.11690251E+01	.72113501E-00	14.50	.41688118E-01	.83522010E-02
4.60	.10997910E+01	.66451489E-00	15.00	.37776578E-01	.73222308E-02
4.70	.10359400E+01	.61336107E-00	16.00	.31308974E-01	.56978766E-02
4.80	.97695739E-00	.56705084E-00	17.00	.26239270E-01	.45004040E-02
4.90	.92238649E-00	.52504282E-00	18.00	.22208969E-01	.36019010E-02
5.00	.87182121E-00	.48686509E-00	19.00	.18964547E-01	.29170442E-02
5.20	.78129835E-00	.42040149E-00	20.00	.16323258E-01	.23876302E-02
5.40	.70292912E-00	.36493056E-00	21.00	.14151103E-01	.19731524E-02
5.60	.63473533E-00	.31833677E-00	22.00	.12348297E-01	.16449073E-02
5.80	.57511369E-00	.27896542E-00	23.00	.10839496E-01	.13822211E-02
6.00	.52275528E-00	.24551126E-00	24.00	.95670821E-02	.11699810E-02
6.20	.47658434E-00	.21693655E-00	25.00	.84864819E-02	.99698886E-03
6.40	.43571113E-00	.19241013E-00	26.00	.75628443E-02	.85484367E-03
6.60	.39939537E-00	.17126163E-00	27.00	.67686535E-02	.73717037E-03
6.80	.36701778E-00	.15294689E-00	28.00	.60819880E-02	.63908011E-03
7.00	.33805750E-00	.13702147E-00	29.00	.54852367E-02	.55678696E-03
7.20	.31207438E-00	.12312026E-00	30.00	.49641415E-02	.48733242E-03
7.40	.28869467E-00	.11094173E-00	32.00	.41044906E-02	.37809261E-03
7.60	.26759963E-00	.10023551E-00	34.00	.34325531E-02	.29783344E-03
7.80	.24851631E-00	.90792752E-01	36.00	.28997394E-02	.23779554E-03
8.00	.23121003E-00	.82438403E-01	38.00	.24718101E-02	.19215946E-03
8.20	.21547826E-00	.75025098E-01	40.00	.21241636E-02	.15696983E-03
8.40	.20114560E-00	.68428265E-01	42.00	.18388131E-02	.12948298E-03
8.60	.18805961E-00	.62542173E-01	44.00	.16024006E-02	.10776060E-03
8.80	.17608738E-00	.57276749E-01	46.00	.14048642E-02	.90410427E-04
9.00	.16511269E-00	.52554972E-01	48.00	.12385266E-02	.76417318E-04
9.20	.15503357E-00	.48310760E-01	50.00	.10974613E-02	.65030841E-04

Table 10.3

The "master solution" $\varphi_-(x)$ for $F = -1$

x	$\varphi_-(x)$	$-\varphi_-'(x)$	x	$\varphi_-(x)$	$-\varphi_-'(x)$
.50	.10719112E+05	.11379947E+06	1.04	.38923927E+03	.14934830E+04
.51	.96553759E+04	.99349096E+05	1.06	.36081529E+03	.13518248E+04
.52	.87248454E+04	.87087387E+05	1.08	.33505801E+03	.12264201E+04
.53	.79076132E+04	.76632615E+05	1.10	.31166468E+03	.11150966E+04
.54	.71871994E+04	.67677883E+05	1.12	.29037261E+03	.10160116E+04
.55	.65498881E+04	.59974922E+05	1.14	.27095314E+03	.92759600E+03
.56	.59842058E+04	.53321717E+05	1.16	.25320662E+03	.84850951E+03
.57	.54805088E+04	.47552980E+05	1.18	.23695826E+03	.77760307E+03
.58	.50306538E+04	.42532761E+05	1.20	.22205458E+03	.71388860E+03
.59	.46277352E+04	.38148680E+05	1.22	.20836048E+03	.65651379E+03
.60	.42658725E+04	.34307405E+05	1.24	.19575670E+03	.60474128E+03
.61	.39400387E+04	.30931067E+05	1.26	.18413776E+03	.55793138E+03
.62	.36459200E+04	.27954425E+05	1.28	.17341009E+03	.51552758E+03
.63	.33798018E+04	.25322588E+05	1.30	.16349053E+03	.47704449E+03
.64	.31384742E+04	.22989194E+05	1.32	.15430501E+03	.44205766E+03
.65	.29191548E+04	.20914938E+05	1.34	.14578741E+03	.41019507E+03
.66	.27194237E+04	.19066378E+05	1.36	.13787857E+03	.38112981E+03
.67	.25371705E+04	.17414962E+05	1.38	.13052549E+03	.35457404E+03
.68	.23705492E+04	.15936233E+05	1.40	.12368058E+03	.33027372E+03
.69	.22179406E+04	.14609176E+05	1.45	.10852082E+03	.27797809E+03
.70	.20779208E+04	.13415676E+05	1.50	.95718385E+02	.23556936E+03
.71	.19492343E+04	.12340076E+05	1.55	.84835224E+02	.20089755E+03
.72	.18307717E+04	.11368803E+05	1.60	.75526988E+02	.17233691E+03
.73	.17215500E+04	.10490058E+05	1.65	.67520540E+02	.14864519E+03
.74	.16206965E+04	.96935600E+04	1.70	.60597411E+02	.12886398E+03
.75	.15274347E+04	.89703267E+04	1.75	.54581491E+02	.11224713E+03
.76	.14410721E+04	.83124912E+04	1.80	.49329789E+02	.98208864E+02
.77	.13609900E+04	.77131479E+04	1.85	.44725406E+02	.86285663E+02
.78	.12866345E+04	.71662211E+04	1.90	.40672170E+02	.76108035E+02
.79	.12175088E+04	.66663536E+04	1.95	.37090484E+02	.67379400E+02
.80	.11531664E+04	.62088119E+04	2.00	.33914098E+02	.59860140E+02
.82	.10372636E+04	.54044146E+04	2.05	.31087579E+02	.53355467E+02
.84	.93615905E+03	.47248262E+04	2.10	.28564312E+02	.47706115E+02
.86	.84758856E+03	.41476903E+04	2.15	.26304907E+02	.42781144E+02
.88	.76968818E+03	.36551588E+04	2.20	.24275938E+02	.38472340E+02
.90	.70091442E+03	.32328868E+04	2.25	.22448910E+02	.34689830E+02
.92	.63998214E+03	.28692721E+04	2.30	.20799440E+02	.31358623E+02
.94	.58581580E+03	.25548748E+04	2.35	.19306579E+02	.28415865E+02
.96	.53751083E+03	.22819704E+04	2.40	.17952265E+02	.25808651E+02
.98	.49430296E+03	.20442050E+04	2.45	.16720871E+02	.23492269E+02
1.00	.45554359E+03	.18363248E+04	2.50	.15598827E+02	.21428786E+02
1.02	.42067999E+03	.16539651E+04	2.60	.13637022E+02	.17936013E+02

Table 10.3

(continued)

x	$\varphi_-(x)$	$-\varphi_-'(x)$	x	$\varphi_-(x)$	$-\varphi_-'(x)$
2.70	.11988996E+02	.15123863E+02	8.80	.25580293E-00	.91598536E-01
2.80	.10594693E+02	.12839684E+02	9.00	.23832214E-00	.83370394E-01
2.90	.94072987E+01	.10969222E+02	9.20	.22239470E-00	.76044125E-01
3.00	.83899628E+01	.94259915E+01	9.40	.20785213E-00	.69503824E-01
3.10	.75134145E+01	.81438328E+01	9.60	.19454739E-00	.63650578E-01
3.20	.67542096E+01	.70716453E+01	9.80	.18235177E-00	.58399684E-01
3.30	.60934234E+01	.61696000E+01	10.00	.17115224E-00	.53678361E-01
3.40	.55156689E+01	.54063907E+01	10.50	.14688680E-00	.43800806E-01
3.50	.50083496E+01	.47572158E+01	11.00	.12699133E-00	.36091255E-01
3.60	.45610886E+01	.42022811E+01	11.50	.11052608E-00	.30003510E-01
3.70	.41652857E+01	.37256791E+01	12.00	.96783487E-01	.25145259E-01
3.80	.38137733E+01	.33145423E+01	12.50	.85223982E-01	.21230490E-01
3.90	.35005463E+01	.29583979E+01	13.00	.75431269E-01	.18047833E-01
4.00	.32205481E+01	.26486728E+01	13.50	.67080702E-01	.15439119E-01
4.10	.29695010E+01	.23783103E+01	14.00	.59916603E-01	.13284616E-01
4.20	.27437696E+01	.21414717E+01	14.50	.53735764E-01	.11492729E-01
4.30	.25402519E+01	.19333022E+01	15.00	.48375318E-01	.99926890E-02
4.40	.23562895E+01	.17497464E+01	16.00	.39613837E-01	.76592245E-02
4.50	.21895962E+01	.15874011E+01	17.00	.32843945E-01	.59682342E-02
4.60	.20381983E+01	.14433988E+01	18.00	.27530933E-01	.47187990E-02
4.70	.19003862E+01	.13153135E+01	19.00	.23303405E-01	.37795947E-02
4.80	.17746741E+01	.12010846E+01	20.00	.19897953E-01	.30626657E-02
4.90	.16597663E+01	.10989555E+01	21.00	.17124247E-01	.25078089E-02
5.00	.15545300E+01	.10074238E+01	22.00	.14842449E-01	.20730055E-02
5.20	.13692170E+01	.85117247E-00	23.00	.12948258E-01	.17284087E-02
5.40	.12121269E+01	.72400042E-00	24.00	.11362807E-01	.14524770E-02
5.60	.10780980E+01	.61966028E-00	25.00	.10025718E-01	.12294359E-02
5.80	.96305899E-00	.53341376E-00	26.00	.88902387E-02	.10475795E-02
6.00	.86377012E-00	.46162955E-00	27.00	.79197850E-02	.89811500E-03
6.20	.77763170E-00	.40149767E-00	28.00	.70854550E-02	.77436261E-03
6.40	.70254152E-00	.35082413E-00	29.00	.63642108E-02	.67119526E-03
6.60	.63678744E-00	.30788148E-00	30.00	.57375368E-02	.58463942E-03
6.80	.57896553E-00	.27129889E-00	32.00	.47106816E-02	.44959090E-03
7.00	.52791740E-00	.23998059E-00	34.00	.39147662E-02	.35136040E-03
7.20	.48268152E-00	.21304457E-00	36.00	.32883859E-02	.27853774E-03
7.40	.44245535E-00	.18977630E-00	38.00	.27887237E-02	.22363200E-03
7.60	.40656554E-00	.16959339E-00	40.00	.23853055E-02	.18160614E-03
7.80	.37444431E-00	.15201841E-00	42.00	.20560419E-02	.14900001E-03
8.00	.34561069E-00	.13665783E-00	44.00	.17846561E-02	.12339069E-03
8.20	.31965541E-00	.12318561E-00	46.00	.15589758E-02	.10305198E-03
8.40	.29622875E-00	.11133031E-00	48.00	.13697746E-02	.86734581E-04
8.60	.27503071E-00	.10086486E-00	50.00	.12099732E-02	.73521338E-04

the series converges, but so slowly that it cannot be summed numerically in a straightforward manner, especially if only a limited number of coefficients is available. A second even more vexing problem, which we also met, is that of finding a numerical "sum" to a power series altogether outside its circle of convergence. By "sum" we mean here: the value of the analytic continuation of the function which inside the circle of convergence is represented by the power series. This seems to be the most reasonable definition. An example is furnished by the geometric series $1 + z + z^2 + \dots$; here the "sum" in the above sense would be defined as $(1-z)^{-1}$, even for $|z| \geq 1$.

To solve these problems one can apply the so-called "e_k-transforms", a family of sequence-to-sequence transformations discussed extensively by Shanks [5]. Though as yet not very deeply founded, these transforms do yield remarkably accurate numerical results of the type required in the situations sketched above. For examples, discussions and proofs the reader is referred to Shanks' article; here only a brief survey of the most important features is presented.

Definition:

let S_n , $n = 0, 1, \dots$ be any sequence (often, but not necessarily, the partial sums of a power series). The "k-th order transform" of S_n is defined as

$$e_k(S_n) = \frac{\begin{vmatrix} S_{n-k} & S_{n-k+1} & \cdots & S_n \\ \Delta S_{n-k} & \Delta S_{n-k+1} & \cdots & \Delta S_n \\ \vdots & \vdots & & \vdots \\ \Delta S_{n-1} & \Delta S_n & \cdots & \Delta S_{n+k-1} \end{vmatrix}}{\begin{vmatrix} 1 & 1 & \cdots & 1 \\ \Delta S_{n-k} & \Delta S_{n-k+1} & \cdots & \Delta S_n \\ \vdots & \vdots & & \vdots \\ \Delta S_{n-1} & \Delta S_n & \cdots & \Delta S_{n+k-1} \end{vmatrix}} \quad , \quad (10.2.1)$$

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5) D. Shanks, J.Math. & Phys. 34 (1955) 1-42.

where $\Delta S_n = S_{n+1} - S_n$; if both numerator and denominator of (10.2.1) vanish, then

$$e_k(S_n) = e_{k-1}(S_n) ; \qquad (10.2.2)$$

the definition is completed by

$$e_0(S_n) = S_n \quad . \qquad (10.2.3)$$

A very important property of e_k is the following:

if

$$\left.\begin{aligned} S_n &= S + \sum_{i=1}^{k} a_i q_i^n \quad , \\ \text{then} \quad e_k(S_n) &= S \quad , \end{aligned}\right\} \qquad (10.2.4)$$

irrespective of the values of the q_i . If all $|q_i| < 1$, then obviously $\lim_{n\to\infty} S_n = S$; in this case the e_k -transform has accelerated the convergence to the extent of giving the limit at once. If one or more $|q_i| \geq 1$, the limit of S_n does not exist, but application of e_k still yields a number. Shanks introduces the name "anti-limit" for the value S obtained in this case; it corresponds to the "sum" of a divergent series as discussed above. This property indicates which transform must be applied in a given situation. For the geometric series, for instance, one can write

$$S_n = \frac{1-z^{n+1}}{1-z} = \frac{1}{1-z} - \frac{z}{1-z} z^n \quad , \qquad (10.2.5)$$

which is of the form (10.2.4) with $k=1$. Therefore application of e_1 yields $(1-z)^{-1}$ regardless of the magnitude of $|z|$. Similarly, $[(1-z)(2-z)]^{-1}$ can be written in the form (10.2.4) with two terms, and application of e_2 to the partial sums of its series expansion will give the exact value in one operation.

In general, however, application of e_k will not yield an exact value. One can follow two courses:

(i) Form the sequences S_n , $e_1(S_n)$, $e_2(S_n)$, ... , $e_k(S_n)$; in general each successive sequence will diverge less strongly, and eventually converge faster, than its predecessor.

(ii) Form the sequences S_n, $e_1(S_n)$, $e_1(e_1(S_n)) \equiv e_1^2(S_n)$, ..., $e_1^m(S_n)$, applying e_1 repeatedly to the same sequence.

We mention one property of the "m-fold repeated transform" e_1^m which is particularly important for numerical applications: if $e_1^m(S_n)$ and $e_1^{m+1}(S_n)$ both tend to a limit as $n \to \infty$, then these limits are the same, and $e_1^{m+1}(S_n)$ converges faster than $e_1^m(S_n)$. When applying these transforms repeatedly, one must be careful; for it is possible that for isolated values of the independent variable [5] one arrives at a value which is not equal to the "sum" defined above. To make sure that this phenomenon, of which Shanks gives an example, does not occur, it is advisable to compare the values obtained with some independent results.

As an example we summed the Baker series (4.5. 2) at $x = 1$ (its radius of convergence $x_0 \approx .44$). Application of e_1^m yields the value $\varphi(1) = .4240080521$. As a check (4.4. 4), which does converge, was calculated with $B = -1.5880710226$: this yields the same value to 10 significant figures. An algorithm to calculate $e_k(S_n)$ and an estimate of the errors in the results will be given in appendix 10.31.

10.3 . Indispensable algorithms

10.31. Wynn's algorithm for e_k ; error estimates

The definition (10.2.1) is rather impractical to calculate $e_k(S_n)$ since it involves the calculation of two $(k+1)\times(k+1)$ determinants for each term of the sequence, and all the work has to be repeated for every new transform one wants to calculate. Wynn [6] developed an algorithm particularly suited for numerical application on a digital computer. Introducing a set of auxiliary quantities $\varepsilon_p(S_n)$ by

$$\begin{aligned} \varepsilon_{2m}(S_n) &\equiv e_m(S_n) \quad , \\ \varepsilon_{2m+1}(S_n) &\equiv \left[\bar{e}_m(\Delta S_n)\right]^{-1} \quad , \end{aligned} \tag{10.31.1}$$

he shows that

$$\varepsilon_p(S_n) = \varepsilon_{p-2}(S_n) + \frac{1}{\varepsilon_{p-1}(S_{n+1}) - \varepsilon_{p-1}(S_{n+1-1})} \quad , \tag{10.31.2}$$

6) P. Wynn, M.T.A.C. 10 (1956) 91-6; here we have adapted Wynn's notation to conform to Shanks' definition of e_k .

where $q = \frac{1}{2}\left[1 - (-1)^k\right]$.

When applying $e_k(S_n)$ we normally adopted as the "sum" of the series $e_k(S_n)$ for the highest values n and k reached; when applying e_1^m then $e_1^m(S_n)$ for the highest available n and m . If S_n^k denoted this value, we assumed as error estimate the quantity

$|S_n^k - S_{n-1}^k|$ if S_n was an oscillating sequence and

$|S_n^k - S_{n+1}^{k-1}|$ if S_n was a monotonous sequence. These estimates turn out to be conservative: in practice there are indications that the real errors involved are less than those estimated.

10.32. Newton's method of successive approximations in two variables

We want to find the root (x_0, y_0) of the equations

$$F(x,y) = 0 \quad , \quad G(x,y) = 0 \quad . \tag{10.32.1}$$

Suppose that an approximate solution (x_k, y_k) is available. Then expanding $F(x,y)$ and $G(x,y)$ as Taylor series around (x_k, y_k) and retaining only the terms linear in $(x-x_k)$ or $(y-y_k)$ one obtains a better approximation (x_{k+1}, y_{k+1}) :

$$\begin{aligned} x_{k+1} &= x_k - \frac{F G_y - G F_y}{F_x G_y - G_x F_y} \quad , \\ y_{k+1} &= y_k - \frac{F G_x - G F_x}{F_y G_x - G_y F_x} \quad , \end{aligned} \tag{10.32.2}$$

where all function values are evaluated at (x_k, y_k) . Here the convergence of this algorithm is assumed. If the equations (10.32.1) can be separated in the form

$$f_1(x) = g_1(y) \quad ; \quad f_2(x) = g_2(y) \quad , \tag{10.32.3}$$

one has similarly

$$\begin{aligned} x_{k+1} &= x_k - \frac{(f_1 - g_1) g_2' - (f_2 - g_2) g_1'}{f_1' g_2' - f_2' g_1'} \quad , \\ y_{k+1} &= y_k - \frac{(g_1 - f_1) f_2' - (g_2 - f_2) f_1'}{g_1' f_2' - g_2' f_1'} \quad , \end{aligned} \tag{10.32.4}$$

where again the right-hand-sides are evaluated for (x_k, y_k).

10.33. Expansion of a power series, raised to an arbitrary power

Suppose that

$$f(x) = \sum_{i=0}^{\infty} f_i x^i \quad , \quad g(x) = \sum_{i=0}^{\infty} g_i x^i \qquad (10.33.1)$$

where $g(x) = [f(x)]^p$.

The problem is to find g_i from f_i . Differentiating the relation between $g(x)$ and $f(x)$ leads to

$$x\, g'(x)\, f(x) = p\, x\, f'(x)\, g(x) \qquad (10.33.2)$$

Writing out the coefficient of x^i in (10.33.2) yields

$$\sum_{j=0}^{i} f_j\, (i-j)\, g_{i-j} = p \sum_{j=0}^{i} j\, f_j\, g_{i-j} \quad . \qquad (10.33.3)$$

Hence we find the algorithm [7]:

$$g_0 = f_0^p \; ; \text{ for } i \geq 1 \; , \; g_i = \frac{1}{i f_0} \sum_{j=1}^{i} [(p+1)j - i]\, f_j\, g_{i-j} \quad . \qquad (10.33.4)$$

Similarly, if

$$g(x) = \ln f(x) \qquad (10.33.5)$$

then

$$g_0 = \ln f_0 \; ; \text{ for } i \geq 1 \; , \; g_i = \frac{1}{i f_0} \left[i f_i - \sum_{j=1}^{i-1} (i-j)\, f_j\, g_{i-j} \right] . \qquad (10.33.6)$$

In two variables, if

$$\left.\begin{aligned} f(x,y) &= \sum_{i,j=0}^{\infty} f_{i,j}\, x^i y^j \; , \\ g(x,y) &= \sum_{i,j=0}^{\infty} g_{i,j}\, x^i y^j \; , \\ g &= f^p \; , \end{aligned}\right\} \qquad (10.33.7)$$

then analogously

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7) H.E. Fettis, Communications A.C.M., March 1963, 104 (CACM algorithm 158).

$$g_{0,0} = f_{0,0}^{p} \quad ;$$

$$i\, f_{0,0}\, g_{i,j} = \sum_{\substack{k=0 \\ k,\ell \neq 0,0}}^{i} \sum_{\ell=0}^{j} [(p+1)k - i]\, f_{k,\ell}\, g_{i-k,j-\ell} \quad , \quad i \neq 0 \, ;$$

$$j\, f_{0,0}\, g_{i,j} = \sum_{\substack{k=0 \\ k,\ell \neq 0,0}}^{i} \sum_{\ell=0}^{j} [(p+1)\ell - j]\, f_{k,\ell}\, g_{i-k,j-\ell} \quad , \quad j \neq 0 \, . \tag{10.33.8}$$

10.34. Derivatives of a power of a function, in terms of the derivatives of the function itself

Suppose two functions $f(x)$ and $g(x)$ are related by

$$g(x) = [f(x)]^{p} \tag{10.34.1}$$

We want to know the derivatives

$$g^{(m)}(e) = \left[\frac{d^m g}{dx^m} \right]_{x=e} \tag{10.34.2}$$

in terms of the derivatives

$$f^{(m)}(e) = \left[\frac{d^m f}{dx^m} \right]_{x=e} \quad , \tag{10.34.3}$$

for a given fixed value $x = e$.

Defining

$$\eta_{\ell,m} = \frac{d^m}{dx^m} [f(x)]^{p-\ell} \tag{10.34.4}$$

and noting the identity

$$\frac{d^m}{dx^m} [f(x)]^{p-\ell} = \frac{d^{m-1}}{dx^{m-1}} \{ (p-\ell) [f(x)]^{p-\ell-1} f^{(1)}(x) \} \, , \tag{10.34.5}$$

one immediately obtains the following algorithm :

$$\left.
\begin{aligned}
&\text{let} \quad \eta_{\ell,0} = [f(e)]^{p-\ell} \quad , 0 \leq \ell \leq \ell_{max} \, ; \\
&\text{and for} \quad 1 \leq k \leq \ell_{max} \quad , \quad 0 \leq \ell \leq \ell_{max} - k \, , \\
&\qquad \eta_{\ell,k} = (p-\ell) \sum_{i=0}^{k-1} \binom{k-1}{i} \eta_{\ell+1,i} \, f^{(k-i)}(e) \, ; \\
&\text{then} \\
&\qquad g^{(m)}(e) = \eta_{0,m} \quad , \quad 1 \leq m \leq \ell_{max} \, .
\end{aligned}
\right\} \tag{10.34.6}$$

10.35. **Expansion of a function of two variables, if one of these is a function of the other**

Let us assume a function of two variables

$$F(x,y) = \sum_{k,l=0}^{\infty} F_{k,l}\, x^k y^l \quad , \tag{10.35.1}$$

and let us also assume that y depends on x in the form

$$y(x) = \sum_{i=0}^{\infty} y_i\, x^i \quad . \tag{10.35.2}$$

Then we want to find the coefficients in the expansion in x alone

$$F(x,y(x)) = \sum_{i=0}^{\infty} F^{(i)}\, x^i \quad , \tag{10.35.3}$$

in terms of the (known) coefficients $F_{k,l}$ and y_i.
In a recursive, computer-oriented manner the solution is formulated as follows:

define functions $$f_k(y) = \sum_{l=0}^{\infty} F_{k,l}\, y^l \quad , \tag{10.35.4}$$

such that $$F(x,y) = \sum_{k=0}^{\infty} x^k f_k(y) \quad . \tag{10.35.5}$$

Form the Taylor expansion of $f_k(y)$ around y_0 :

$$f_k(y) = \sum_{m=0}^{\infty} \frac{1}{m!} f_k^{(m)}(y_0)\,(y-y_0)^m \quad . \tag{10.35.6}$$

Define the coefficients $h_{j,m}$ of the expansion of $(y-y_0)^m$ in powers of x by

$$\left[\sum_{i=0}^{\infty} y_{i+1}\, x^i\right]^m \equiv \sum_{j=0}^{\infty} h_{j,m}\, x^j \quad , \tag{10.35.7}$$

where one can apply section 10.33 to calculate $h_{j,m}$.
For compactness, write

$$a_{k,m} = \frac{1}{m!} f_k^{(m)}(y_0) \quad , \tag{10.35.8}$$

and suppose that these quantities can be calculated from the defining relation (10.35.4) or otherwise (cf. section 6.31). Then by substituting (10.35.6-8) into (10.35.5) and collecting powers of x one finds that

$$F^{(i)} = \sum_{k=0}^{i} \sum_{j=0}^{i-k} a_{i-j-k,k}\; b_{j,k} \quad . \tag{10.35.9}$$

10.36. Continued fraction representation and Padé approximants of a function whose power series expansion is given

Our aim is to find the Padé approximants to a power series expansion of a function

$$f(x) = \sum_{i=0}^{\infty} f_i\, x^i \quad , \tag{10.36.1}$$

if the coefficients f_i are given. To solve this problem, recall that [8] the (n,n) and $(n,n+1)$ approximants are the $(2n)$th and the $(2n+1)$th approximant to the continued fraction representation

$$f(x) = e_0 + \cfrac{x}{e_1 + \cfrac{x}{e_2 + \cfrac{x}{\ddots}}} \quad . \tag{10.36.2}$$

Thus the problem is reduced to that of finding the elements e_j of the continued fraction from the coefficients f_i of the power series.

If one defines functions

$$\varphi_j(x) = e_j + \cfrac{x}{e_{j+1} + \cfrac{x}{e_{j+2} + \cfrac{x}{\ddots}}} \quad , \tag{10.36.3}$$

it is immediately obvious that

$$\left.\begin{aligned} \varphi_j(x) &= e_j + \frac{x}{\varphi_{j+1}(x)} \quad , \\ \text{while} \quad \varphi_j(0) &= e_j \quad \text{and} \quad \varphi_0(x) \equiv f(x) \quad . \end{aligned}\right\} \tag{10.36.4}$$

Thus one arrives at the algorithm:

$$\left.\begin{aligned} &\text{let} \quad a_i^{(0)} = f_i \quad \text{for} \quad i = 0, 1, 2, \ldots \; ; \\ &\text{for} \quad j = 0, 1, 2, \ldots \quad \text{let} \quad \sum_{i=0}^{\infty} a_i^{(j+1)} x^i \equiv \Big[\sum_{i=0}^{\infty} a_{i+1}^{(j)} x^i\Big]^{-1} \; ; \\ &\text{then} \quad a_0^{(j)} = e_j \quad . \end{aligned}\right\} \tag{10.36.5}$$

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8) H.S. Wall, Analytic theory of continued fractions, Van Nostrand, New York-Toronto-London (1948).

For the second stage the algorithm of section 10.33 is applied.

To obtain the Padé approximants one defines polynomials $P_n(x)$, $Q_n(x)$ by

$$\left.\begin{aligned} P_{-1} &= 1 \quad , \quad P_0 = c_0 \quad , \quad P_n = c_n P_{n-1} + x P_{n-2} \; ; \\ Q_{-1} &= 0 \quad , \quad Q_0 = 1 \quad , \quad Q_n = c_n Q_{n-1} + x Q_{n-2} \; . \end{aligned}\right\} \qquad (10.36.6)$$

Then $(n,n) = P_{2n} / Q_{2n}$ and $(n, n+1) = P_{2n+1} / Q_{2n+1}$. (10.36.7)

The $(n, n+\ell)$ approximant, where $\ell > 1$, is easily found by writing

$$f(x) = \sum_{i=0}^{\ell-1} f_i x^i + x^\ell f^*(x) \; , \qquad (10.36.8)$$

determining the (n,n) approximant to $f^*(x)$ by means of (10.36.5-7), substituting this for $f^*(x)$ in (10.36.8) and bringing the resulting rational function under a common denominator.

The $(n+\ell, n)$ approximant is found as the inverse of the $(n, n+\ell)$ approximant to $[f(x)]^{-1}$.

10.4 . Some integrals of chapter 8

10.41. Integrals of the form $I_{s,t} = \int z^s (z+\alpha)^t dz$

In these integrals the exponents s and t are simultaneously integers or half-odd-integers; they also obey the conditions

$$s > -1 \quad , \quad s + t \geq -1 \; . \qquad (10.41.1)$$

The case where s and t are both integers is straightforward; convenient expansions are

$$I_{s,t} = \sum_{p=0}^{t} \binom{t}{p} \frac{\alpha^p \, z^{s+t+1-p}}{s+t+1-p} \qquad \text{for} \quad t \geq 0 \; ; \qquad (10.41.2)$$

$$I_{s,t} = \sum_{\substack{p=0 \\ p \neq s+t+1}}^{s} \binom{s}{p} \frac{(-\alpha)^p (z+\alpha)^{s+t+1-p}}{s+t+1-p} + \binom{s}{-t-1} (-\alpha)^{s+t+1} \ln(z+\alpha)$$

$$\text{for} \quad t \leq -1 \; . \qquad (10.41.3)$$

When s and t are both half-integer it is possible to reduce $I_{s,t}$ to a sum of terms of the form $z^{s'}(z+\alpha)^{t'}$, together with $I_{-\frac{1}{2},-\frac{1}{2}}$; the latter is

$$I_{-\frac{1}{2},-\frac{1}{2}} = 2\ \mathrm{arsinh}\left(\frac{z}{\alpha}\right)^{\frac{1}{2}} \equiv 2\ln\left[\left(\frac{z}{\alpha}\right)^{\frac{1}{2}} + \left(1+\frac{z}{\alpha}\right)^{\frac{1}{2}}\right]. \qquad (10.41.4)$$

The relations which effect this reduction are most easily derived from the obvious relation $I_{s,t} = I_{s+1,t-1} + \alpha I_{s,t-1}$; after integration by parts and subsequent rearrangement of terms one obtains

$$I_{s,t} = \frac{z^{s+1}(z+\alpha)^{t}}{s+t+1} + \frac{\alpha t}{s+t+1} I_{s,t-1} ,$$

or (10.41.5)

$$I_{s,t} = \frac{z^{s}(z+\alpha)^{t+1}}{s+t+1} - \frac{\alpha s}{s+t+1} I_{s-1,t} .$$

For $t \geq -\frac{1}{2}$ two equivalent expressions are found, analogous to (10.41.2):

$$I_{s,t} = \sum_{p=0}^{s-\frac{1}{2}} \frac{s!\,(s+t-p)!}{(s-p)!\,(s+t+1)!} (-\alpha)^{p} z^{s-p} (z+\alpha)^{t+1}$$
$$+ (-)^{s+\frac{1}{2}} \frac{s!}{(-\frac{1}{2})!} \sum_{p=s+\frac{1}{2}}^{s+t} \frac{t!\,(s+t-p)!}{(s+t+\frac{1}{2}-p)!\,(s+t+1)!} \alpha^{p} z^{\frac{1}{2}} (z+\alpha)^{s+t+\frac{1}{2}-p}$$
$$+ 2\frac{t!}{(-s-1)!\,(s+t+1)!} \alpha^{s+t+1} \mathrm{arsinh}\left(\frac{z}{\alpha}\right)^{\frac{1}{2}} , \qquad (10.41.6a)$$

or

$$I_{s,t} = \sum_{p=0}^{t-\frac{1}{2}} \frac{t!\,(s+t-p)!}{(t-p)!\,(s+t+1)!} \alpha^{p} z^{s+1} (z+\alpha)^{t-p}$$
$$+ (-)^{t+\frac{1}{2}} \frac{t!}{(-\frac{1}{2})!} \sum_{p=t+\frac{1}{2}}^{s+t} \frac{s!\,(s+t-p)!}{(s+t+\frac{1}{2}-p)!\,(s+t+1)!} (-\alpha)^{p} z^{s+t+\frac{1}{2}-p} (z+\alpha)^{\frac{1}{2}}$$
$$+ 2\frac{t!}{(s-1)!\,(s+t+1)!} \alpha^{s+t+1} \mathrm{arsinh}\left(\frac{z}{\alpha}\right)^{\frac{1}{2}} . \qquad (10.41.6b)$$

For $t < -\frac{1}{2}$ a different expression holds, analogous to (10.41.3):

$$I_{s,t} = \sum_{p=0}^{s+t} \frac{s!\,(s+t-p)!}{(s-p)!\,(s+t+1)!}\,(-\alpha)^p\, x^{s-p}\,(x+\alpha)^{t-1} + 2\,\frac{t!}{(-s-1)!\,(s+t+1)!}\,\alpha^{s+t+1}\left[\operatorname{arsinh}\left(\frac{x}{\alpha}\right)^{\frac{1}{2}} - \sum_{q=1}^{-t-\frac{1}{2}} \frac{x^{q-\frac{1}{2}}\,(x+\alpha)^{-q+\frac{1}{2}}}{2q-1}\right]. \tag{10.41.7}$$

10.42. Integrals of the form $J_{s,t} = \int x^s (x+\alpha)^t \operatorname{arsinh}(x/\alpha)^{\frac{1}{2}}\,dx$

The conditions on s and t are again given by (10.41.1). In a way analogous to that adopted to derive (10.41.5) one arrives at the recurrence relations

$$J_{s,t} = \frac{x^{s+1}\,(x+\alpha)^t}{s+t+1} \operatorname{arsinh}\left(\frac{x}{\alpha}\right)^{\frac{1}{2}} + \frac{\alpha t}{s+t+1}\,J_{s,t-1} - \frac{1}{2(s+t+1)}\,I_{s+\frac{1}{2},\,t-\frac{1}{2}}$$

and (10.42.1)

$$J_{s,t} = \frac{x^s\,(x+\alpha)^{t+1}}{s+t+1} \operatorname{arsinh}\left(\frac{x}{\alpha}\right)^{\frac{1}{2}} - \frac{\alpha s}{s+t+1}\,J_{s-1,\,t} - \frac{1}{2(s+t+1)}\,I_{s-\frac{1}{2},\,t+\frac{1}{2}}\,.$$

With the help of (10.42.1) any $J_{s,t}$ can be reduced to either $J_{-\frac{1}{2},-\frac{1}{2}}$ or $J_{0,-1}$, together with $I_{s',t'}$ which are known from the previous section. We will not carry out the reduction explicitly here. One finds immediately that

$$J_{-\frac{1}{2},-\frac{1}{2}} = \left[\operatorname{arsinh}\left(\frac{x}{\alpha}\right)^{\frac{1}{2}}\right]^2, \tag{10.42.2}$$

while a convenient expansion for $J_{0,-1}$ is [9]

$$J_{0,-1} = \left[\ln 2\left(1+\frac{x}{\alpha}\right)^{\frac{1}{2}}\right]^2 + 2\left[\frac{1}{2^3}\,\frac{\alpha}{x+\alpha} + \frac{1\cdot 3}{2\cdot 4^3}\left(\frac{\alpha^2}{x+\alpha}\right)^2 + \cdots\right]. \tag{10.42.3}$$

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9) See e.g. H.B. Dwight, Tables of Integrals and Other Mathematical Data, 4th Ed. (1961) MacMillan, New York, equation 733.1.