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A DIRECT INVERSION OF THE INTEGRAL EQUATION OF TRANSFER

by

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FOREWORD

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2(d) 1. Introduction

In the Eddington approximation, to which we restrict attention in this section, the integral equation for the line source function in the case of complete redistribution, no continuous opacity, and a plane parallel semi-infinite geometry, may be written

\[ S(\tau) = \lambda b + \frac{\tilde{\omega}_0 \sqrt{3}}{2 \sqrt{\pi}} \int_0^\infty S(t) K(t - \tau) \, dt \]  \hspace{1cm} (2d.1)

with

\[ K(t - \tau) = \int_{-\infty}^\infty e^{-2\tau^2} \exp(-\sqrt{3} |t - \tau| e^{-\mathbf{v}^2}) \, d\mathbf{v} \]  \hspace{1cm} (2d.2)

The physical meanings of the terms in the equation are described by Jeffries (Ref. 1). It should be noted that no restriction is placed on the depth (i.e., \( \tau \)) variation of \( \lambda \), \( b \), or \( \tilde{\omega}_0 \) (\( = 1 - \lambda \)).

The transfer equation (2d.1) is the integral form with the appropriate boundary condition of the differential equation

\[ \frac{1}{3} \frac{d^2 J_\nu}{d\tau^2} = J_\nu - S \]  \hspace{1cm} (2d.3)

where

\[ S = \tilde{\omega}_0 \int J_\nu \phi_\nu \, d\nu + \lambda b \]  \hspace{1cm} (2d.4)

and where \( \phi_\nu = e^{-\nu^2 / \sqrt{\pi}} \) is the profile of the (assumed Gaussian) absorption coefficient while \( J_\nu \) is the mean intensity in the spectral line at frequency \( \nu \) Doppler widths from the line center. The quantity \( b(\tau) \) is related to the rates of transitions (other than direct upward
or downward radiative transitions in the line itself) which populate and depopulate the two levels involved in the line. In the particular case of a two-level atom b(τ) reduces to the Planck function B(T) at the local temperature; in more general cases this no longer necessarily applies.

A fast, reliable method for solving this equation is essential for progress in the study of the excitation of a multilevel atom in conditions which depart from local thermodynamic equilibrium. In such cases a simple analysis shows that we shall have to solve one equation of the above basic type for each spectral line or continuum formed by the atom. Since the parameters λ and b, and the transformations from optical depth scales from line to line, are dependent on the source functions in the other lines, the solution of this multilevel problem (the so-called case of "interlocking") reduces to the solution of a system of coupled integral equations. In any real case this system will have to be solved iteratively. To be feasible even on a fast computer, a scheme for a rapid solution is essential.

The difficulty encountered in practice with the solution of equation (2d,1) is that for a strong spectral line in a tenuous gas (as a stellar atmosphere) the quantity λ is very small (for example λ~10^{-6} for L_α in the solar chromosphere) so that ̂ω_α is very close to unity and the integral equation is almost singular. As a result the direct replacement of the integral by a quadrature sum leads to an ill-conditioned set of linear equations while any simple iterative approach has such slow convergence as to be impracticable as a method of solution.

In this section of the report we shall describe a direct method for the solution of equation (2d,1) which has been found to differ by no more than a few percent from the solution of the corresponding differential equation. The procedure itself is simple but quite impracticable for anything other than a fast computer.
It might be wondered why, in such a necessarily elaborate study, one should start with an approximate equation of transfer when the exact integral equation differs only in that the factors $\sqrt{3}$ in equation (2d.1) are set equal to unity and the exponential function involving $|t-\tau|$ in the kernel is replaced by the first exponential integral. At the time the investigation began, adequate solutions for $S(\tau)$ had only been obtained from the Eddington approximation to the differential equation by the method of Jefferies and Thomas (Ref. 2). The chief reason for using the Eddington approximation here is, therefore, that we then have a means of testing the accuracy of a solution of the integral equation. The basic difficulty of solving the equation lies, in any case, not in the form of the kernel -- which can be easily enough changed -- but in the smallness of $\lambda$. Finally, throughout the most important part of the atmosphere it has been shown that the Eddington approximation is generally good to at least a few percent and the physical meaning of the solutions will not be influenced by its adoption.

2(d) 2. A Method of Solution

A method for solving the integral equation can be centered around the expansion

$$S(t) = \sum_{i=1}^{n} a_i e^{-k_i t}$$

(2d.5)

in which the exponents $k_i$ are chosen and the coefficients $a_i$ are to be determined. Substituting the form (2d.5) into the equation (2d.1), we obtain the following equations for the coefficients $a_i$:

$$\sum_{i=1}^{N} a_i \left[ \lambda e^{-k_i \tau} - \frac{\omega_0}{\pi} G(\tau, k_i) \right] = \lambda b$$

(2d.6)

where

$$G(\tau, k) = \frac{\sqrt{3}}{\sqrt{\pi}} \int_{0}^{\infty} \frac{dve^{-2v^2}}{(k^2 - 3e^{-2v^2})^2} \left\{ (k + \sqrt{3}e^{-v^2}) \exp(-\sqrt{3}e^{-v^2}) - \frac{2k^2v^2 - k\tau}{\sqrt{3}} \right\}.$$
The unknowns $a_1$ are then to be found by a least square solution of equation (2d.6) at a number of values of $\tau$. This simple scheme forms the basis of the method used here—some refinements have been necessary, however, and these are discussed below. The proper selection of the $k_i$ and the optical depths $\tau_j$ at which the equations (2d.6) are to be solved is, of course, a critical aspect of the method. Some insight into this question may be obtained as follows.

For large $\tau$, $K|t-\tau|$ acts roughly as a delta function so that equation (2d.1) becomes

$$S(\tau) \cong \lambda b + \omega_o \frac{S(\tau)\sqrt{3}}{2\sqrt{\pi}} \int_0^\infty K|t-\tau|dt$$

(2d.8)

or, on evaluating the integral,

$$S(\tau) \cong \lambda b/\left[\lambda + \frac{\omega_o}{2\sqrt{\pi}} \int_{-\infty}^\infty e^{-v^2} \exp(-\sqrt{3} \tau e^{-v^2})dv\right]$$

(2d.9)

which for large $\tau$ and small $\lambda$ reduces to the approximate form

$$S(\tau) \cong b/(1 + 5 \times 10^{-2}/\tau\lambda).$$

(2d.10)

Thus $S(t)$ saturates to within about 5% of the value $b$ at $\tau \sim 1/\lambda$ and the smallest value of $k$ must therefore be rather smaller than $\lambda$ while the largest depth at which we attempt to solve the system should be greater than $\lambda^{-1}$. In fact we have chosen $\tau_{\text{max}} = 10\lambda^{-1}$. All cases so far studied were for $\lambda$ independent of depth; in a variable $\lambda$ problem some similar simple rule could easily be formulated.

Having chosen a $\tau_{\text{max}}$ in this way the remaining $\tau$ for which equations (2d.6) are to be solved were assigned according to the sequence

$$0.7 \tau_{\text{max}}, 0.4 \tau_{\text{max}}, 0.2 \tau_{\text{max}}, 0.1 \tau_{\text{max}}, \text{etc.,}$$

continuing down to a minimum $\tau$ which was generally set equal to $10^{-3}$. The $k$ values were chosen from the sequence $4 \times 10^p; 1.5 \times 10^p$ (with $p$ integral) and
the largest and smallest $k$ for any particular problem were set by the requirements

$$
1 \leq k_{\text{max}} \tau_{\text{max}} < 3
$$

$$
0.01 < k_{\text{min}} \tau_{\text{min}} < 0.1
$$

(2d.11)

In this way it was hoped to provide the basic functions $\exp(-k\tau)$ with sufficient flexibility to match any likely variation in $S(\tau)$.

2(d) 3. A Modification

It was found impossible to apply directly the above simple procedure over the full range of $\tau$ (typically $10^{-3}$ to $10^7$), since this required too many unknowns $a_i$ to give a stable solution. This total optical depth range was therefore split into two-decade subranges (e.g., $10^7$ to $10^5$, $10^5$ to $10^3$ ... etc.) within each of which coefficients $a_i$ were separately sought. In the first range (i.e., the one at greatest depth) the expansion form was chosen in the slightly different form

$$
S(\tau) = b(\tau) + \sum a_ie^{-k_i\tau}
$$

(2d.12)

in order to conform to the known\(^1\) variation of $S$ at great depths. Although clearly sufficient, it has not, so far, been determined whether or not this step was necessary to produce a stable solution with the correct behavior at large depths.

A difficulty now arises of matching the solutions from one subrange in $\tau$ to the next. To a certain extent this can be overcome by requiring that the slopes and values of $S(\tau)$ should match across the

\(^1\)Provided the scale of the depth variations of $b(\tau)$ is greater than $\lambda^{-1}$. In other words, it is not generally true that $S(\tau) \sim b(\tau)$, for this to be so the radiation must be able to follow its own sources.
boundary between two subranges—however, some care must be exercised to see that these conditions are not so heavily weighted in the least square equations as to dominate the matrix or so underweighted that they are ignored. We attempted to ensure this by a rough normalization to unity of the dominant terms in the conditional equations used to form the least squares set.

Some algebraic details arising in the procedure are given in Appendix I; the general method is clear enough and, perhaps rather surprisingly, seems to lead to a stable system of equations. An unsatisfactory aspect lies in the need to split the integration range into sections; this arises essentially because of the specific form chosen to represent $S(\tau)$. However, the method does seem to work well enough for our needs although refinements could undoubtedly be made. The fact that the method works at all is of some interest. An extensive search of current summaries turned up no method which was of the slightest value in solving the integral equation for the case $\lambda < 10^{-2}$.

2(d) 4. Numerical Examples

Clearly the solution will be the more difficult, the smaller is $\lambda$. Figure 1 shows a solution for $\lambda = 10^{-6}$, $b = 1$; the solid line shows $S(\tau)$ derived from the differential equation; the plotted points compare the solution for the same problem obtained via the integral equation. The procedure is clearly good, giving answers correct to a percent or so over ranges of $10^3$ in $S(\tau)$ and about $10^{10}$ in $\tau$. A much more severe test was made, again for $\lambda = 10^{-6}$, with $b$ varying according to the law

$$b(\tau) = 1 + 200 \exp(-10^{-5} \tau) .$$

(2d.13)

---

2 In a ninth-order Gaussian quadrature approximation to the frequency integral; cf. Jefferies and Thomas (Ref. 2).
The comparison between the differential and integral equation solutions for this case is shown in Figure 2; it is quite satisfactory but, as expected, is not as good as for the b constant case. A natural and simple extension would be to iterate on these approximate solutions; but this has not been done as yet.

2(d) 5. Conclusions

In this section of the report we have described a direct method for the solution of integral equations of Fredholm's second kind, to an accuracy of order one percent, for cases when \( \lambda > 10^{-6} \). Smaller values of \( \lambda \) have not yet been properly tested but there seems no indication at \( \lambda = 10^{-6} \) that the method is about to fail--the relative accuracy at \( \lambda = 10^{-6} \) being equal to that at \( \lambda = 10^{-4} \). The method clearly lacks a great deal in sophistication; our interest, however, was in finding some method which worked rather than in studying the mathematical structure of the integral equation.

A great deal more work remains; so far no attempt has been made in this procedure to incorporate a Voigt function form for the absorption coefficient. As shown by Avrett and Hummer in Ref. 3 of this report, this can greatly influence the variation of \( S \) with \( \tau \). In addition it would be desirable to modify equation (2d.1) to the exact form.
FIGURE CAPTIONS

Figure 1. Comparison between the solution of the integral equation (points) and that of the corresponding differential equation (complete curve) for the isothermal case; $\epsilon = 10^{-6}$.

Figure 2. Comparison between the solution of the integral equation (points) and that of the corresponding differential equation (complete curve) for an atmosphere with variable $b$; $\epsilon = 10^{-6}$. 
APPENDIX I

ALGEBRAIC DETAILS OF THE SOLUTION
OF THE INTEGRAL EQUATION OF TRANSFER

(1) Analysis

In the case when b is independent of depth, the expansion for
S(t) in the deepest layer was chosen in the form

$$S(t) = b + \sum a_i e^{-k_i t}$$  \hspace{1cm} (A1.1)

so that the equations for the $a_i$ become

$$\sum a_i \left\{ \lambda e^{-k_i t} - \omega G(k_i, t) \right\} + \omega b A(t) = 0$$  \hspace{1cm} (A1.2)

in which the function G is given by equation (2d. 7) of the text while

$$A(t) = \frac{1}{\sqrt{\pi}} \int_0^\infty e^{-v^2} \exp(-\sqrt{3} t e^{-v^2}) \, dv$$  \hspace{1cm} (A1.3)

It may be noted that

$$A(t) = -G(0, t)$$  \hspace{1cm} (A1.4)

As explained in the text, the simple form (A1.2) could not be used
over the entire range of depth and it was found necessary to introduce
separate expansions over each of a set of subranges in $\tau$. Within each
of these we again fitted $S(t)$ with a sum of exponentials.

In detail the procedure ran as follows: By the method given in
the text a value of $\tau_{max}$ was assigned, the expansion (A1.1) assumed,
the exponents $k_i$ chosen as given in the text, and the coefficients of
the resulting set of additional equations \((A1.2)\) were computed at the depths \(0.7 \tau_{\max}, 0.4 \tau_{\max}, 0.2 \tau_{\max} \ldots \) down to \(10^{-3} \tau_{\max}\). From these a least square set was found and solved for the coefficients \(a_i\) after the equations had been weighted by the procedure given in paragraph (2) below.

We next assumed that, over the range \(10^{-2} \tau_{\max} > t > 0\), the source function could be represented by the expansion

\[
S(t) = \sum b_i e^{-k'_i t} \tag{A1.5}
\]

while in the range \(t > 10^{-2} \tau_{\max}\) \(S(t)\) was given by the form \((A1.1)\) in which the \(a_i\) were now known from the preceding step. In this case the equations for the \(b_i\) are

\[
\sum b_i \left\{ e^{-k'_i t} - \tilde{\omega} G(k'_i, t) + \tilde{\omega} e^{-k'_i t} D(k'_i, \tau_1 - t) \right\} = \lambda b + \tilde{\omega} \sum a_i e^{-k_1 \tau_1} D(k_1, \tau_1 - \tau) + \tilde{\omega} b A(\tau_1 - t) \tag{A1.6}
\]

in which \(\tau_1 = 10^{-2} \tau_{\max}\) and

\[
D(k, \tau) = \frac{\sqrt{3}}{\sqrt{\pi}} \int_0^\infty e^{-2v^2} \exp(-\sqrt{\frac{3}{\pi}} v e^{-v^2}) \frac{e^{-\sqrt{3} x e^{-v^2}}}{k + \sqrt{3} e^{-v^2}} \, dv. \tag{A.7}
\]

The coefficients of \(b_i\) and the constant term were computed, again for the series of depths \(0.7 \tau_1, 0.4 \tau_1, \ldots, 10^{-3} \tau_1\), while the \(k'_i\) were again chosen by the method indicated in the text by taking \(\tau_{\max} = \tau_1\) and \(\tau_{\min} = 10^{-3} \tau_1\).

Additional conditions on the coefficients \(b_i\) were applied by requiring that, at \(t = \tau_1\), the values of \(S(t)\) and the slopes should match. That is, we required that
\[ b + \sum a_i e^{-k_i \tau_1} = \sum b_i e^{-k_i' \tau_1} \]  \hspace{1cm} \text{(A1.8)}

and

\[ \sum k_i a_i e^{-k_i \tau_1} = \sum k_i' b_i e^{-k_i' \tau_1}. \]  \hspace{1cm} \text{(A1.8')} 

The equations (A1.6) and (A1.8) are independent and the coefficients of the unknowns \( b_i \) can vary over large ranges. To ensure that they have more or less equal weight we adopted the scaling factors given in paragraph 2 below.

The rest of the computation follows the same pattern. In the range \( 10^{-4} \tau_{\text{max}} > t > 0 \) we assumed the expansion

\[ S(t) = \sum c_i e^{-k_i'' t}. \]  \hspace{1cm} \text{(A1.9)}

In the range \( 10^{-4} \tau_{\text{max}} < t < 10^{-2} \tau_{\text{max}} \) we used the expansion (A1.5) with the (now known) coefficients \( b_i \) and for \( t > 10^{-2} \tau_{\text{max}} \) we used the expansion (A1.1). The equations for the \( c_i \) take the form

\[ \sum c_i \left\{ \lambda e^{-k_i'' t} - \tilde{\omega}_o G(k_i', t) + \tilde{\omega}_o e^{-k_i'' \tau_2} D(k_i', \tau_2 - t) \right\} \]

\[ = \lambda b + \tilde{\omega}_o \sum a_i e^{-k_i \tau_1} D(k_i, \tau_1 - t) + \tilde{\omega}_o \sum b_i \left\{ e^{-k_i' \tau_1} D(k_i', \tau_1 - t) - e^{-k_i' \tau_2} D(k_i', \tau_2 - t) \right\} + \tilde{\omega}_o b A(\tau_1 - t) \]  \hspace{1cm} \text{(A1.10)}

with \( \tau_2 = 10^{-4} \tau_{\text{max}} \). The \( k_i'' \), and the \( t \) at which these equations were to be solved, were again chosen as in the text with \( \tau_{\text{max}} = \tau_2 \) and \( \tau_{\text{min}} = 10^{-3} \tau_2 \).
The extension of the equations (A1.10) to the subsequent ranges is straightforward; in general, the procedure was carried out down to \( \tau = 10^{-3} \) by which time \( S(t) \) had essentially reached its surface \( (t = 0) \) value.

(2) **The Scaling Factors**

**Equations (A1.6)**

If the value of the upper division point \( (\tau_1 \text{ in this case}) \) exceeds 2, the equations (A1.6) were scaled by \( 10t \). This has the effect of making the dominant coefficients in the equations of the same general size. If the value of the upper division point is less than 2, the equations (A1.6) were not weighted.

**Equations (A1.8)**

The slope equation (A1.8') was weighted by \( k_{\text{min}}^{-2} \) multiplied by the scale factor for equation (A1.8). This latter factor was chosen as unity in the first \( (\tau > \tau_1) \) and second depth ranges and as \( 10^{-3}/\sqrt{\lambda} \) in the third and subsequent ranges.

These empirical rules can be justified on grounds of plausibility, yet they form a most unsatisfactory part of the procedure and a more objective weighting method to be sought.

(3) **Extensions**

(a) **Arbitrary \( b(\tau) \)**

In the first range (i.e., largest \( \tau \)) we chose the representation

\[
S(\tau) = b - \sum a_i e^{-k_i \tau}
\]

for \( b \) constant, but if \( b \) depends on \( \tau \) different terms arise from the integral term of the integral equation. The easiest way to handle these is probably to expand \( b \) as a series of exponentials--the relevant integrals
can then be carried out, at least partially, as above. In the case
treated in Section II(d), equation (2d.13), the procedure was straightforward and need not be repeated here.

(b) Iteration

Further programming is required before iteration is possible. In principle the method is simple enough; we merely use the fitting constants $a_i$ determined in the first approximation (or the preceding iteration) to compute the constants in the conditional equations for the least squares set. However until the relative weighting of the equations is better understood this step may be premature.

(c) Multilevel problems

Simultaneous integral equations arising in multilevel transfer problems can be solved by the same general procedure. So far this has not been undertaken.

(4) Computation of the Integrals and Some Comments on the Numerical Method

The integrals occurring in the analysis require delicate handling and some brief discussion of the methods used in their evaluation is desirable. The integrals are time consuming to evaluate and a great saving in time was effected by computing them once for a wide range for $k$ and $\tau$, storing them on tape and interpolating as needed. Since the integrals vary tremendously in value as $k$ and $\tau$ vary over their ranges $(10^3 - 10^{-8}; 10^8 - 10^{-3})$, interpolation is only satisfactory in terms of a suitably scaled function which takes out the major variations in the integrals. For this purpose we need approximate values of the integrals--these are discussed below.

(a) The A Integral

This integral, which is the simplest to discuss, is defined as
\[ A(t) = \frac{1}{\sqrt{\pi}} \int_0^\infty e^{-v^2} \exp\left(-\sqrt{3} \cdot t \cdot e^{-v^2}\right) \, dv. \]  \hspace{1cm} (A1.12)

The maximum value of the integrand occurs at \( v = 0 \) if \( \sqrt{3} \cdot t < 1 \)
or at \( v = \sqrt{\ln \sqrt{3} \cdot t} \) if \( \sqrt{3} \cdot t > 1 \). Approximate values of the integral are

\[ A(t) \sim 1/2 \hspace{3cm} \sqrt{3} \cdot t < 1 \]
\[ A(t) \sim \left[t \sqrt{\ln \sqrt{3} \cdot t}\right]^{-1} \hspace{3cm} \sqrt{3} \cdot t > 1 \]  \hspace{1cm} (A1.13)

(b) **The D Integral**

This is defined as

\[ D(k,t) = \frac{\sqrt{3}}{\sqrt{\pi}} \int_0^\infty \frac{e^{-2v^2}}{(k + \sqrt{3} \cdot e^{-v^2})} \exp\left(-\sqrt{3} \cdot t \cdot e^{-v^2}\right) \, dv. \]  \hspace{1cm} (A1.14)

Approximate values for the integral can be obtained by considering limiting forms for \( k \) and \( t \) large or small compared to unity. In this way we find up to a constant of proportionality:

\[ D(k,t) \propto \frac{1}{\sqrt{2 \cdot k + \sqrt{3}}} \hspace{3cm} \sqrt{3} \cdot t \ll 1 \]  \hspace{1cm} (A1.15)
\[ D(k,t) \sim \frac{1}{t(kt + 1)^{1/2} \cdot \sqrt{\ln t} \cdot \sqrt{3}} \hspace{3cm} \sqrt{3} \cdot t \gg 1 \]

(c) **The G Integral**

In contrast to the A and D integrals which are always positive, the G integral changes sign quite rapidly for certain combinations of \( k,t \). Its variation with \( k \) and \( t \) can be found, by studying limiting cases from its definition

\[ G(k,t) = \frac{\sqrt{3}}{\sqrt{\pi}} \int_0^\infty \frac{e^{-2v^2}}{(k + \sqrt{3} \cdot e^{-v^2})} \exp\left(-\sqrt{3} \cdot t \cdot e^{-v^2} - \frac{2k^2}{\sqrt{3} \cdot e^{-v^2} \cdot e^{-kt}}\right) \, dv. \]  \hspace{1cm} (A1.16)
We obtained the following results:

(i) $\sqrt{3} t > 1, \; kt > 1$

$$G(k,t) \propto [kt^2 \sqrt{kn} t^{\sqrt{3}}]^{-1} \quad (A1.17)$$

(ii) $\sqrt{3} t < 1 < kt$

$$G(k,t) \propto k^{-1} \left[ 1 - \frac{2\sqrt{2}k}{\sqrt{3}} e^{-kt} \right] \quad (A1.18)$$

(iii) $kt < 1 < \sqrt{3}t$

$$G(k,t) \propto \left( t \sqrt{kn^{\sqrt{3}} t} \right)^{-1} \left[ 1 - 2(kt)^2 e^{-kt} \right] \quad (A1.19)$$

(iv) $kt < 1, \sqrt{3} t < 1$

$$G(k,t) \sim -1 \quad (A1.20)$$

In all cases the proportionality constant is positive and of order unity.

These limiting forms are rather more delicate than those discussed for the A and D integrals. We have not attempted to determine interpolated forms applicable in the region where the sign change occurs. As can be seen from equations (A1.17) through (A1.20) this occurs at about $kt = 1$ for $\sqrt{3} t \gg 1$ and, for $\sqrt{3} t \ll 1$ at

$$\frac{2\sqrt{2}k}{\sqrt{3}} e^{-kt} = 1 \quad (A1.21)$$

The limiting forms for each of the integrals have been checked against the computed values; they agree well in all cases.

To evaluate the integrals it was first necessary to determine the range of $v$ giving the dominant contribution. This was done by determining the approximate value $v_{\text{max}}$ at which the integrand was a maximum and then the two values $0 < v_1 < v_{\text{max}}$, $v_2 > v_{\text{max}}$ at which the
integrand was down by a factor $10^8$ from its maximum. The range $v_2 - v_1$ was then divided into a large number (100 to 200) of equal intervals and the integral computed by Simpson's rule.

For interpolation, the integrals were first scaled by dividing by their approximate values given above—thus yielding a much more slowly varying function. Interpolation in the A and D tables presents no problem; however, since the G integral changes sign more care must be taken with it. When the values of $k$ and $t$ were such that the integral was close to a sign change the interpolation was bypassed as too inaccurate and the integral was computed in full.
REFERENCES

