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An exact method for the evaluation of the S matrix for the Yukawa potential problem

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Abstract. The S matrix problem for the Yukawa potential is studied. The radial Schrödinger equation is Laplace transformed into a retarded ordinary differential equation (RODE). As a consequence of an asymptotic treatment it is shown that S_l is related *exactly* to the values of the transformed function at $l+1$ points on the complex plane. The treatment of the RODE by means of a *convergent* numerical scheme permits an estimate of S_l to any order of precision.

1. Introduction

For the Yukawa potential scattering problem it is known that the bounded solution of the pertinent Schrödinger equation:

$$\frac{\mathrm{d}^2u(r)}{\mathrm{d}r^2}+\left(k^2+\lambda\frac{\exp(-r/a)}{r}-\frac{l(l+1)}{r^2}\right)u(r)=0, \qquad r>0, \tag{1.1}$$

has the asymptotic property:

$$u(r)=A\sin(kr-\tfrac{1}{2}l\pi+\delta_l)+\mathrm{o}(1) \qquad \text{for } r\to+\infty. \tag{1.2}$$

Here $S_l=\exp(2\mathrm{i}\delta_l)$ is usually referred to as the 'S matrix' and δ_l as the 'phase shift' (Newton 1966). In the literature (Hulthèn 1944, Gerjouy and Saxon 1954, Mower 1955, Swan 1960a, b, Wojtczak 1963) approximate methods and numerical schemes have appeared which concern the evaluation of the phase shifts or of related quantities. In this paper we present an *exact* procedure for the computation of S_l and δ_l: more precisely, with the help of a Laplace transform procedure we construct a numerical scheme (with step size h) which is convergent to S_l for $h\to0^+$ for each choice of k, λ, a, l (with $k>0, \lambda>0, a>0, l$ non-negative integer). Our treatment hinges on the fundamental properties which connect the behaviour of a function $y(\xi)$ for $\xi\to+\infty$ with the behaviour of its Laplace transform,

$$\hat{y}(s)=\mathscr{L}[y(\xi)]=\int_0^\infty \exp(-s\xi)y(\xi)\,\mathrm{d}\xi,$$

in the neighbourhood of its rightmost complex-plane singularities. Appendix 1 is devoted—following Doetsch (1955)—to a precise formulation of these properties.

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Martin (1959, 1960) has employed the Laplace transform procedure to study the analyticity properties of S_l as a function of k. However, as far as we know, integral transform methods have not been applied to the problem of the actual evaluation of the S matrix for the Yukawa potential. As a matter of fact, in the extensive literature which concerns quantum mechanical problems and the Schrödinger equation, the integral transform method has *not* been used with great frequency. This is remarkable since the technique provides reliable and reasonably simple computational procedures†. It has been recommended and employed by Schrödinger himself in his first paper on wave mechanics‡. In the late 1940s the integral transform method has been applied to several problems in quantum mechanics by Kallmann and Päsler (1949a, b, 1950, and references quoted therein). Finally Doetsch has reconsidered the relevant case of the hydrogen atom in his landmark *Handbuch* (Doetsch 1955, §§ 7.3 and 15.3).

As coauthor of a recent paper (Paiano and Picca 1975) one of us has employed a Laplace transform procedure to treat the S matrix problem for the exponential and the Yukawa potentials in s-partial wave ($l = 0$). The present paper treats the case of the Yukawa potentitial for integer $l \geqslant 0$. We wish to mention that Paiano and Piccccca (1975) study the asymptotic behaviour of the wavefunction for $r \to +\infty$ by an appropriate deformation on the complex plane of the integration path for the inverse transformation. In the present paper simpler results are obtained explicitly by exploiting a connection theorem (from Doetsch 1955) between the asymptotic behaviours. The theorem is quoted in appendix 1. In agreement with recommendations by Doetsch (1955, *Lit. hist. Nachweise* Nos 68, 172, 175, 176) we have made an effort not to rely simply on a formal (heuristic) analysis but rather to establish our asymptotic results on the basis of a rigorous treatment. Unfortunately this has required a somewhat cumbersome procedure. However the detailed treatment presented here—aside from being the required mathematical justification for the results that concern the Yukawa potential—will also be employed in future work for the treatment of problems involving other choices of the potential (such as, e.g., the case of the superposition of exponential and Yukawa potentials).

The contents of the paper are organised as follows. In § 2 the S matrix problem is formulated. After a change of variables and after Laplace transforming, a difference-differential equation on the half-plane $\{\mathrm{Re}(s) > 0\}$ is obtained which in turn is equivalent to a Volterra integral equation. After an analytical continuation of $\hat{y}(s) = \mathscr{L}[\xi^{-(l+1)}u(\xi)]$ (where $\xi = r/a$) on the strip $\{-1 < \mathrm{Re}(s) \leqslant 0\}$ the behaviour of $\hat{y}$ in the neighbourhood of its rightmost singular points, $s = \mathrm{i}k_0$, $s = -\mathrm{i}k_0$ (where $k_0 = ka$) is studied and the pertinent parameters are examined: it is shown that they are related to a linear combination of $\hat{y}$ and its first l derivatives evaluated at $\mathrm{i}k_0 + 1$; in turn these quantities can be expressed as linear combinations of $\hat{y}(\mathrm{i}k_0+1)$, $\hat{y}(\mathrm{i}k_0+2) \ldots \hat{y}(\mathrm{i}k_0+l+1)$. Then theorem 2 of appendix 1 can be applied to evaluate the S matrix. In § 3 the problem of the calculation of $\hat{y}(\mathrm{i}k_0+R)(R = 1, 2, \ldots, l+1)$ is then tackled. We

† '*Bei der Anwendung der $\mathscr{L}$-Traaransformation auf Differentialgleichungen erhält man oft $\mathscr{L}$-Transformierte, deren Originalfunktionen $F(t)$ nicht bekannt, d.h. nicht durch klassische Funktionen darstellbar sind. In solchen Fällen ist die asymptotische Entwicklung oft das einzige Mittel, um überhaupt etwas über $F(t)$ aussagen zu können* (*Doetsch* 1955, *p.* 172).

‡ '*Die Integraldarstellung gestattet nicht nur, das asymptotische Verhalten der Gesamtheit von Lösungen, wenn r in bestimmter Weise ins Unendliche geht, zu überlicken, sondern auch, dieses Verhalten für eine bestimmte Lösung anzugeben, was immer viel schwieriger ist*' (*Schrödinger* 1926, *reprinted in Schrödinger* 1928, 1963).

Here Schrödinger indicates with '*Integraldarstellung*' the inverse transformation integral.

find that $\hat{y}$ obeys a retarded oidinary differential equation for which, after an appropriate change of variables, the numerical procedure of Feldstein (1964) can be applied (the same procedure has been applied by Paiano and Picca 1975). In § 4 the results are summarised and a comparison is made between the 'exact' values for phase shifts and cross sections and the corresponding estimates which have appeared in the literature. As we mentioned appendix 1 is devoted to a summary of the pertinent results from the asymptotic theory of the Laplace transformation. Appendix 2 summarises Feldstein's treatment, which is still unpublished.

2. The analytical treatment

2.1. Problem statement

After the change of variables $\xi = r/a$, $k_0 = ka$, $\lambda_0 = \lambda a$ and $y = \xi^{-(1+l)}u$, we can formulate the Yukawa potential problem (equations (1.1), (1.2) above) as follows: seek a function y such that

$$\left(\xi\frac{\mathrm{d}^2}{\mathrm{d}\xi^2}+2(l+1)\frac{\mathrm{d}}{\mathrm{d}\xi}+k_0^2\xi+\lambda_0\,\mathrm{e}^{-\xi}\right)y(\xi)=0, \qquad \xi\in(0,+\infty) \qquad (2.1a)$$

$$y\in C^\infty((0,+\infty),\mathbb{R}) \qquad (2.1b)$$

$$\sup\{|\xi^{1+l}y(\xi)|:\xi\in(0,\infty)\}<+\infty \qquad (2.1c)$$

$$y(0^+)=y^0\in\mathbb{R}-\{\mathrm{o}\}. \qquad (2.1\mathrm{d})$$

The following proposition summarises well known results (Newton 1966, §11.1, Olver 1974, chap. 12, § 6.1, Coppel 1965).

Proposition 1. For assigned values of λ_0, k_0, y^0, l (with $\lambda_0>0$; $k_0>0$; $y^0\in\mathbb{R}-\{\mathrm{o}\}$; l non-negative integer) problem 1 admits the unique solution

$$u(\xi)=y^0\sum_{R=0}^{\infty}a_R\xi^{R+l+1}, \qquad \xi\in(0,+\infty), \qquad (2.2)$$

where

$$a_0=1 \qquad (2.3a)$$

$$a_R=-(\mathscr{I}(R+l+1))^{-1}\sum_{j=0}^{R-1}\beta_{R-j}a_j, \qquad R\in\{1,2\ldots\} \qquad (2.3b)$$

provided

$$\mathscr{I}(\eta)=\eta(\eta-1)-l(l+1), \qquad (2.4a)$$

$$k_0^2\xi^2+\lambda_0\exp(-\xi)-l(l+1)=\sum_{R=0}^{\infty}\beta_R\xi^R, \qquad \xi\in(0,+\infty). \qquad (2.4b)$$

The series which appear on the right-hand sides of equations (2.2) and (2.4b) have unbounded radii of convergence. Moreover, on the set $[0,\pi)\times(\mathbb{R}-\{0\})$ there is an unique pair (δ_l, A) such that, if we let

$$u_\infty(\xi)=\tfrac{1}{2}A[\![\exp\{\mathrm{i}[k_0\xi+\delta_l-\tfrac{1}{2}(l+1)\pi]\}+\exp\{-\mathrm{i}[k_0\xi+\delta_l-\tfrac{1}{2}(l+1)\pi]\}]\!]$$
$$=A\sin(k_0\xi+\delta_l-\tfrac{1}{2}l\pi), \qquad (2.5)$$

then

$$y(\xi)=y^0\xi^{-(1+l)}(u_\infty(\xi)+o(1)), \qquad \text{for } \xi\to+\infty, \tag{2.6a}$$

$$\frac{d}{d\xi}y(\xi)=y^0\xi^{-(1+l)}\Big(\frac{d}{d\xi}u_\infty(\xi)+o(1)\Big), \qquad \text{for } \xi\to+\infty, \tag{2.6b}$$

$$\frac{d^2}{d\xi^2}y(\xi)=y^0\xi^{-(1+l)}\Big(\frac{d^2}{d\xi^2}u_\infty(\xi)+o(1)\Big), \qquad \text{for } \xi\to+\infty. \tag{2.6c}$$

Here A, δ_l may depend on λ_0, k_0, l; but they are independent of ξ and y^0. Finally, positive parameters K_0, K_1, K_2 exist such that

$$|y^0|K_0=\sup\{|y(\xi)|:\xi\in(0,+\infty)\}<+\infty, \tag{2.7a}$$

$$|y^0|K_1=\sup\{|dy/d\xi|:\xi\in(0,+\infty)\}<+\infty, \tag{2.7b}$$

$$|y^0|K_2=\sup\{|d^2y/d\xi^2|:\xi\in(0,+\infty)\}<+\infty. \tag{2.7c}$$

The main purpose of this paper is the evaluation of the 'S matrix', i.e.

$$S_l=\exp(2i\delta_l) \tag{2.8}$$

as a function of k_0, λ_0, l. We shall also provide an estimate for the 'error term', $y(\xi)-\xi^{-(1+l)}u_\infty(\xi)$, as $\xi\to+\infty$. Remembering that the parameters A, δ_l to be computed are y^0 independent, we find it convenient to let

$$y^0=-1/(2l+1). \tag{2.9}$$

2.2. *The Laplace transformed problem*

On account of equations (2.5), (2.1*a*), (2.7*a*), (2.6*a*) we can claim that the Laplace integral

$$\hat{y}(s)=\mathscr{L}[y(\xi)]=\int_0^\infty \exp(-s\xi)y(\xi)\,d\xi \tag{2.10}$$

converges absolutely to an analytic function for $\mathrm{Re}(s)>0$; does not exist for $\mathrm{Re}(s)\leqslant 0$. since y is real valued, the reflection principle

$$\hat{y}(\bar{s})=\bar{\hat{y}}(s), \qquad \mathrm{Re}(s)>0, \tag{2.11}$$

holds (here a bar denotes complex conjugation). Moreover, on account of equations (2.1*b*), (2.1*d*), (2.7*a*) and (2.7*b*), integrating by parts we find

$$|s\hat{y}(s)|\leqslant|y^0|+\left|\int_0^\infty \exp(-s\xi)\frac{d}{d\xi}y(\xi)\,d\xi\right|\leqslant|y^0|\Big(1+\frac{K_1}{\beta}\Big), \qquad \mathrm{Re}(s)\geqslant\beta>0. \tag{2.12}$$

Finally, integrating by parts and making use of equation (2.1*d*), (2.7), we find:

$$\mathscr{L}\Big[\frac{d}{d\xi}y(\xi)\Big]=s\hat{y}(s)-y^0, \qquad \mathrm{Re}(s)>0;$$

$$\mathscr{L}\Big[\xi\frac{d^2}{d\xi^2}y(\xi)\Big]=-2s\hat{y}(s)-s^2\frac{d}{ds}\hat{y}(s)+y^0, \qquad \mathrm{Re}(s)>0;$$

$$\mathscr{L}[\xi y(\xi)]=-\frac{d}{ds}\hat{y}(s), \qquad \mathrm{Re}(s)>0;$$

$$\mathscr{L}[\exp(-\xi)y(\xi)] = \hat{y}(s+1), \qquad \operatorname{Re}(s) > -1.$$

Then we can claim that the Laplace transform (2.10) of the unique solution y of equations (2.1), (2.9) is a solution of the problem

$$\left((s^2+k_0^2)\frac{\mathrm{d}}{\mathrm{d}s} - 2ls\right)\hat{y}(s) = 1 + \lambda_0\hat{y}(s+1), \qquad \operatorname{Re}(s) > 0, \tag{2.13a}$$

$$\forall\beta > 0: \quad \hat{y}(s) = \mathrm{O}(s^{-1}), \quad \text{for } |s| \to dz+\infty, \text{ uniformly on } \{\operatorname{Re}(s) \geqslant \beta\} \tag{2.13b}$$

$$\hat{y}(s) \text{ analytic on } \{\operatorname{Re}(s) > 0\} \tag{2.13c}$$

where (2.13b) is a consequence of equation (2.12). For the time being we do not claim that $\hat{y} = \mathscr{L}[y]$ is the *unique* solution of problem (2.13). Now we observe that equation (2.13a) can be written in the equivalent forms

$$\frac{\mathrm{d}}{\mathrm{d}s}\frac{\hat{y}(s)}{(s^2+k_0^2)^l} = \frac{1+\lambda_0\hat{y}(s+1)}{(s^2+k_0^2)^{l+1}}, \qquad \operatorname{Re}(s) > 0, \tag{2.14}$$

and

$$\frac{\hat{y}(\gamma+\mathrm{i}\omega)}{[(\gamma+\mathrm{i}\omega)^2+k_0^2]^l} = \frac{\hat{y}(\gamma+1+\mathrm{i}\omega)}{[(\gamma+1+\mathrm{i}\omega)^2+k_0^2]^l} - \int_\gamma^{\gamma+1}\frac{1+\lambda_0\hat{y}(\tau+1+\mathrm{i}\omega)}{[(\tau+\mathrm{i}\omega)^2+k_0^2]^{l+1}}\,\mathrm{d}\tau, \tag{2.15}$$

with $\gamma \in (0, +\infty)$ and $\omega \in \mathbb{R}$.

Moreover we observe that if we let

$$\mathrm{D}^R\hat{y}(s) = \frac{\mathrm{d}^R}{\mathrm{d}s^R}\hat{y}(s), \qquad R \in \{0, 1, 2, \ldots\}, \tag{2.16}$$

then the difference-differential equation (2.13a) yields

$$\mathrm{D}^1\hat{y}(s) = \frac{1+2ls\hat{y}(s)+\lambda_0\hat{y}(s+1)}{s^2+k_0^2}, \qquad \operatorname{Re}(s) > 0, \tag{2.17a}$$

$$\mathrm{D}^R\hat{y}(s) = \frac{[2s(l-R+1)\mathrm{D}^{R-1}+(R-1)(2l-R+2)\mathrm{D}^{R-2}]\hat{y}(s)+\lambda_0\mathrm{D}^{R-1}\hat{y}(s+1)}{s^2+k_0^2}$$

$$\operatorname{Re}(s) > 0,\ R \in \{2, 3, \ldots\}, \tag{2.17b}$$

so that, as a consequence of equation (2.13b),

$$\mathrm{D}^R\hat{y}(s) = \mathrm{O}(s^{-R-1}), \qquad \text{for } |s| \to +\infty \text{ on } \{\operatorname{Re}(s) \geqslant \beta\}. \tag{2.17c}$$

Finally we find that any function y which satisfies equations (2.13) is a solution of the Volterra problem

$$\frac{\hat{y}(\gamma+\mathrm{i}\omega)}{[(\gamma+\mathrm{i}\omega)^2+k_0^2]^l} = \int_\gamma^{+\infty}\frac{1+\lambda_0\hat{y}(\tau+1+\mathrm{i}\omega)}{[(\tau+\mathrm{i}\omega)^2+k_0^2]^{l+1}}\,\mathrm{d}\tau, \qquad \gamma \in (0, +\infty),\ \omega \in \mathbb{R}, \tag{2.18a}$$

$$\int_\gamma^{+\infty}|\hat{y}(\tau+\mathrm{i}\omega)|^2\,\mathrm{d}\tau < +\infty, \qquad \gamma \in (0, +\infty),\ \omega \in \mathbb{R}. \tag{2.18b}$$

Since the kernel in (2.18a) is of class L^2, a classical result (Courant and Hilbert 1953, chap. 3, § 9, Pogorzelski 1966, chap. 2, §§ 1 and 6) guarantees that (2.18a) admits an unique solution of class (2.18b). Since uniqueness for problem (2.18) implies uniqueness for problem (2.13) we can claim the following proposition.

Proposition 2. The Laplace transform $\hat{y}$ of the unique solution of equation (2.1), (2.9) is the unique solution of equations (2.13) on the half-plane $\{\mathrm{Re}(s)>0\}$.

In § 3 we shall actually employ equation (2.14) to evaluate $\hat{y}$. In this section we are interested in establishing a connection between the behaviour of y for $\xi\to\infty$ and the behaviour of $\hat{y}$ on the neighbourhood of its rightmost singularities. The treatment which follows is related to theorem 2 of appendix 1. Actually the use of theorem 1 would be much simpler. However, for our problem assumption (A.4) would require an 'error' of order $O(\exp(-\epsilon\xi))$ with $\epsilon>0$, whereas result (2.6*a*)—which is taken from the literature—exhibits an 'error' estimate of order $O(\xi^{-1-l})$ which is not sharp enough.

2.3. The analytic continuation of $\hat{y}$ and its asymptotic behaviour for $s\to \mathrm{i}k_0$ and $s\to -\mathrm{i}k_0$

The following pertinent result is a direct consequence of the properties of poles for analytic functions.

Proposition 3. The function $\theta=(s^2+k_0^2)^{-(l+1)}(1+\lambda_0\hat{y}(s+1))$ admits the Laurent expansions

$$\theta(s)=\sum_{R=0}^{\infty} c_R(s-\mathrm{i}k_0)^{R-(l+1)}, \qquad \text{on } C_+=\{s\in\mathbb{C}\colon 0<|s-\mathrm{i}k_0|<b\},$$

$$\theta(s)=\sum_{R=0}^{\infty} \bar{c}_R(s+\mathrm{i}k_0)^{R-(l+1)}, \qquad \text{on } C_-=\{s\in\mathbb{C}\colon 0<|s+\mathrm{i}k_0|<b\},$$

where $b=\min\{1, 2k_0\}$ and

$$c_R=\frac{1}{R!}\lim_{s\to\mathrm{i}k_0}\left(\frac{\mathrm{d}}{\mathrm{d}s}\right)^R\frac{1+\lambda_0\hat{y}(s+1)}{(s+\mathrm{i}k_0)^{l+1}}. \tag{2.19}$$

Then, as a consequence of equation (2.14) we can claim m that

$$\frac{\mathrm{d}}{\mathrm{d}s}\frac{\hat{y}(s)}{(s^2+k_0^2)^l}=\theta(s)=(s-\mathrm{i}k_0)^{-(l+1)}\sum_{R=0}^{\infty}c_R(s-\mathrm{i}k_0)^R, \qquad \text{on } W_+=C_+\cap\{\mathrm{Re}(s)>0\}.$$

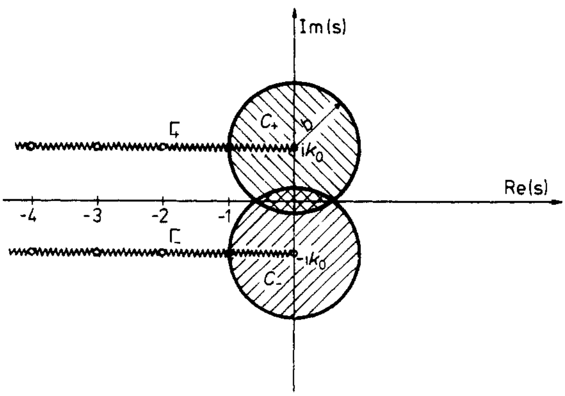

Figure 1. Complex plane analysis of the function $\hat{y}$. For the analytically continued function $\hat{y}$, Γ_+ and Γ_- are branch cuts and the points $\mathrm{i}k_0, \mathrm{i}k_0-1, \mathrm{i}k_0-2, \ldots, -\mathrm{i}k_0, -\mathrm{i}k_0-1, \ldots$ are the branch points. The radius b of the open circles C_+ and C_- is the smallest number among $2k_0$ and 1. The expansions (2.25) hold on C_+-Γ_+ and C_--Γ_- respectively.

Hence term-by-term integration yields the representation

$$\hat{y}(s)=(s+\mathrm{i}k_0)^l\sum_{R=0}^{\infty}w_R(s-\mathrm{i}k_0)^R+(s^2+k_0^2)^l c_l\ln(s-\mathrm{i}k_0)$$

$$=(s+\mathrm{i}k_0)^l\sum_{R=0}^{\infty}w_R(s-\mathrm{i}k_0)^R+c_l\ln(s-\mathrm{i}k_0)$$

$$\times\sum_{\nu=0}^{l}\binom{l}{\nu}(2\mathrm{i}k_0)^{l-\nu}(s-\mathrm{i}k_0)^{l+\nu},\qquad s\in W_+ \tag{2.20a}$$

where $w_R=c_R/(R-l)$ (for $R\neq l$); where w_l is an appropriate complex parameter; and where we require $\ln(p)\in\mathbb{R}$ for $p>0$. Moreover, the symmetric result

$$\hat{y}(s)=(s-\mathrm{i}k_0)^l\sum_{R=0}^{\infty}\bar{w}_R(s+\mathrm{i}k_0)^R+(s^2+k_0^2)^l\bar{c}_l\ln(s+\mathrm{i}k_0)$$

$$=(s-\mathrm{i}k_0)^l\sum_{R=0}^{\infty}\bar{w}_R(s+\mathrm{i}k_0)^R+\bar{c}_l\ln(s+\mathrm{i}k_0)\sum_{\nu=0}^{l}\binom{l}{\nu}(-2\mathrm{i}k_0)^{l-\nu}(s+\mathrm{i}k_0)^{l+\nu} \tag{2.20b}$$

is also valid, for $s\in W_-=C_-\cap\{\mathrm{Re}(s)>0\}$. On account of equation (2.19), equations (2.20) establish a connection between the properties of $\hat{y}$ in the neighbourhood of the singularities $\mathrm{i}k_0$, $-\mathrm{i}k_0$ and its behaviour in the neighbourhood of the regular points $\mathrm{i}k_0+1$, $-\mathrm{i}k_0+1$. Moreover on the right-hand sides of equations (2.20) a regular contribution (which admits a power series representation) and a singular logarithmic contribution can be identified; then a comparison of equations (2.20) with equation (A.1) shows that in the neighbourhood of $\mathrm{i}k_0$, $-\mathrm{i}k_0$, $\hat{y}$ admits an asymptotic representation of class (A.3) with $j=2$ provided $\mathrm{Re}(s)>0$. Now we consider an analytic continuation of $\hat{y}$ on the imaginary axis and on the left half-plane. The presence of the logarithmic term in equations (2.20) suggests that branch cuts should be introduced before attempting the continuation. It is convenient to select the symmetric cuts

$$\Gamma_+=\{s\in\mathbb{C}\colon \mathrm{Im}(s)=+k_0 \text{ and } \mathrm{Re}(s)\leqslant 0\},$$

$$\Gamma_-=\{s\in\mathbb{C}\colon \mathrm{Im}(s)=-k_0 \text{ and } \mathrm{Re}(s)\leqslant 0\}.$$

Now we claim the following proposition.

Proposition 4. Let

$$S_1=\{s\in\mathbb{C}\colon -1<\mathrm{Re}(s)\leqslant 0\}-(\Gamma_+\cup\Gamma_-)=\{s\in\mathbb{C}\colon -1<\mathrm{Re}(s)\leqslant 0 \text{ and } |\mathrm{Im}(s)|\neq k_0\}.$$

Then continuation of $\hat{y}$ on S_1 obeys equations (2.11), (2.13*a*), (2.14), (2.15), (2.17) on $S_1\cup\{\mathrm{Re}(s)>0\}$ and it admits representation (2.20) on the circles $C_+-\Gamma_+$ and $C_--\Gamma_-$.

The proof of this proposition can be organised as follows: first we observe that equation (2.15) indeed defines an analytic function on S_1 which is a continuation of $\hat{y}$ and which obeys equations (2.11), (2.13*a*), (2.14), (2.17) on S_1; next identity theorems can be used to guarantee uniqueness of the analytic continuation on S_1; finally the latter property and the set of arguments which led to equations (2.20) can be employed to extend the validity of equations (2.20) on $C_+-\Gamma_+$ and $C_--\Gamma_-$.

2.4. Asymptotic properties

In connection with equations (2.20) and (A.1), let

$$\hat{g}(s)=\hat{y}(s)-c_l\ln(s-\mathrm{i}k_0)\sum_{\nu=0}^{l}\binom{l}{\nu}(2\mathrm{i}k_0)^{l-\nu}(s-\mathrm{i}k_0)^{l+\nu}$$
$$-\bar{c}_l\ln(s+\mathrm{i}k_0)\sum_{\nu=0}^{l}\binom{l}{\nu}(-2\mathrm{i}k_0)^{l-\nu}(s+\mathrm{i}k_0)^{l+\nu}. \tag{2.21}$$

Here $\hat{g}$ is of class (A.5) with:

$\alpha=0;\quad j=2;\quad s_1=\mathrm{i}k_0;\quad s_2=-\mathrm{i}k_0,$

$\mu=l;\quad n=l;\quad c_{\nu_1}=\bar{c}_{\nu_2}=c_l\binom{l}{\nu}(2\mathrm{i}k_0)^{l-\nu},\quad (\nu\in\{0,1,2,\ldots,l\}).$

We want to verify that all the assumptions of theorem 2 of appendix 1 are satisfied. First we observe that assumption (a) is satisfied with $\alpha=0$ and (b) is satisfied owing to the fact that proposition 4 extends the validity of equation (2.17c) to $s\in S_1$. Next we observe that if we set $\beta=1$ in equation (2.12) we can claim that

$$|\hat{y}(\gamma+\mathrm{i}\omega)|\leqslant\frac{|y^0|}{|\omega|}(K_1+1)\qquad\text{for }\gamma\in[1,+\infty]\text{ and }\omega\in\mathbb{R}.$$

Then, as a consequence of equation (2.15)

$$|\hat{y}(\gamma+\mathrm{i}\omega)|\leqslant|\hat{y}(\gamma+1+\mathrm{i}\omega)|+\int_\gamma^{\gamma+1}\frac{|1+\lambda_0\hat{y}(\tau+1+\mathrm{i}\omega)|}{|\omega^2-k_0^2|}\,\mathrm{d}\tau$$
$$\leqslant\frac{|y^0|}{|\omega|}(K_1+1)\left(1+\frac{\lambda_0}{|\omega^2-k_0^2|}\right)+\frac{1}{|\omega^2-k_0^2|},\qquad\gamma\in[0,1],\omega\in\mathbb{R}.$$

Hence $\hat{y}(s)\to0$ uniformly for $|s|\to+\infty$ on the strip $\{0\leqslant\mathrm{Re}(s)\leqslant1\}$, and assumption (c) is satisfied. Now let us study the function $\hat{g}$ defined by equation (2.21). It is easy to show that $\hat{g}$ is analytic on the whole half-plane $\{\mathrm{Re}(s)>-1\}$; hence it is continuous and admits complex derivatives of all orders there. Requirements (d) and (e) are thus met. Then as a consequence of theorem 2 of appendix 1 we have the main asymptotic result given by the following proposition.

Proposition 5. The unique solution of equations (2.1), (2.9) admits the asymptotic representation

$$y(\xi)=-c_l\exp(\mathrm{i}k_0\xi)\xi^{-1-l}\sum_{\nu=0}^{l}\frac{l!(l+\nu)!}{\nu!(l-\nu)!}(2\mathrm{i}k_0)^{l-\nu}(-1)^{l+\nu}\xi^{-\nu}$$
$$-\bar{c}_l\exp(-\mathrm{i}k_0\xi)\xi^{-1-l}\sum_{\nu=0}^{l}\frac{l!(l+\nu)!}{\nu!(l-\nu)!}(-2\mathrm{i}k_0)^{l-\nu}(-1)^{l+\nu}\xi^{-\nu}+\mathrm{o}(\xi^{-\rho}), \tag{2.22a}$$

for $\xi\to+\infty$, where ρ is any positive parameter and where c_l is given by equation (2.19).

Equation (2.22a) can be written in the equivalent form

$$y(\xi)=2|c_l|\xi^{-1-l}\sum_{\nu=0}^{l}\frac{l!(l+\nu)!}{\nu!(l-\nu)!}(-2k_0)^{l-\nu}\xi^{-\nu}$$

$$\times\sin[k_0\xi-\tfrac{1}{2}(l+\nu)\pi+\arg(c_l)-\tfrac{1}{2}\pi]+o(\xi^{-\rho}),\qquad \text{for } \xi\to+\infty, \tag{2.22b}$$

where, applying the binomial rule to equation (2.19) and employing notation (2.16):

$$c_l=\frac{1}{l!}\lim_{s\to ik_0}\left(\frac{d}{ds}\right)^l\frac{1+\lambda_0\hat{y}(s)}{(s+ik_0)^{l+1}}$$

$$=(2ik_0)^{-l-1}\left[\binom{-l-1}{l}(2ik_0)^{-l}[1+\lambda_0\hat{y}(ik_0+1)]\right.$$

$$\left.+\lambda_0\sum_{R=1}^{l}\binom{-l-1}{l-R}(2ik_0)^{-l+R}\frac{D^R\hat{y}(ik_0+1)}{R!}\right] \tag{2.23}$$

Results (2.22) exhibit the asymptotic behaviour of $y(\xi)$ for $\xi\to+\infty$. Employing equation (2.15) we find that they are improved versions of the classical results (2.5), (2.6a). Moreover, as a consequence of equation (2.8), for the S matrix we have

$$S_l=\exp\{2i[\arg(c_l)-\tfrac{1}{2}\pi]\}=-c_l/\bar{c}_l. \tag{2.24}$$

2.5. *Comments*

Now consider the particular case $\lambda_0=0$, $l\geqslant 0$, $k_0>0$ (physically it corresponds to a free particle). Then problem (2.1) with condition (2.9) has the solution (Abramowitz and Stegun 1964, § 10)

$$y(\xi)=-(2l-1)!!(k_0\xi)^{-l}j_l(k_0\xi), \tag{2.25}$$

where

$$j_l(z)=\left(\frac{\pi}{2z}\right)^{1/2}J_{l+\frac{1}{2}}(z)=z^l\left(-\frac{1}{z}\frac{d}{dz}\right)^l\frac{\sin z}{z}.$$

After some algebraic manipulations we find that results (2.22), which have been obtained subject to the assumption $\lambda_0>0$, actually yield result (2.25) in the limit $\lambda_0\to 0^+$, with the error term (of order $o(\xi^{-\rho})$ with $\rho>0$) actually equal to zero. This corroborates our results. The presence of the Yukawa potential ($\lambda_0>0$) affects the $l+1$ sinusoidal contributions to the wavefunction (which vanish as $\xi^{-\nu}$ with $\nu\in\{0,1,2,\ldots,l\}$ for $\xi\to+\infty$) by multiplying all the amplitudes by the factor

$$\beta_l=\left|(2ik_0)^{2l+1}\binom{-l-1}{l}^{-1}c_l\right|,$$

where c_l obeys equation (2.23), and by adding to the arguments of the sine functions the phase shift $\arg(c_l)$. Moreover, the presence of the Yukawa potential introduces a contribution which vanishes for $\xi\to+\infty$ faster than any law $\xi^{-\rho}$ ($\rho>0$).

We conclude this section by observing that our treatment can be extended to the study of the above mentioned additional contribution. For $\lambda_0>0$ repeating the analysis of § 2.3 to the left of $\mathrm{Re}(s)=-1$ we find that $\hat{y}$ admits an analytical continuation on $\{\mathrm{Re}(s)\leqslant 0\}-(\Gamma_+\cup\Gamma_-)$ with branch-points at ik_0-R, $-iK_0-R$ ($R\in\{0,1,2,\ldots\}$). Hence the error term in equations (2.22) is of order $\exp(-\xi)\sin(\xi+\phi)$. Of course this contribution does not appear if $\lambda_0=0$.

3. The numerical treatment

3.1. The expression of S_l in terms of $\hat{y}(\mathrm{i}k_0+R)$ for $R\in\{1, 2, \ldots, l+1\}$

Equations (2.23), (2.24) permit the evaluation of S_l provided $\hat{y}$ and its first l derivatives are known at $\mathrm{i}k_0+1$. Since equations (2.16), (2.17) can be combined recursively to construct an algorithm for the evaluation of $\mathrm{D}^R\hat{y}(\mathrm{i}k_0+1)$ in terms of $\hat{y}(\mathrm{i}k_0+1), \hat{y}(\mathrm{i}k_0+2)\ldots\hat{y}(\mathrm{i}k_0+R+1)$, it is clear that c_l can be computed as a linear combination of $\hat{y}(\mathrm{i}k_0+1)\ldots\hat{y}(\mathrm{i}k_0+l+1)$. The following diagram sketches the procedure for the computation of $\mathrm{D}^R\hat{y}(\mathrm{i}k_0+1)(R\in\{1, 2, \ldots, l\})$:

$$
\begin{tikzcd}
\hat{y}(\mathrm{i}k_0+1) \arrow[d] \arrow[dd, bend right] & \hat{y}(\mathrm{i}k_0+2) \arrow[dl] \arrow[d] & \hat{y}(\mathrm{i}k_0+3) \arrow[dl] & \ldots & \hat{y}(\mathrm{i}k_0+l+1) \\
\hat{y}'(\mathrm{i}k_0+1) \arrow[d] & \hat{y}'(\mathrm{i}k_0+2) \arrow[dl] & \ldots & \hat{y}'(\mathrm{i}k_0+l) & \\
\hat{y}''(\mathrm{i}k_0+1) & \ldots & \hat{y}''(\mathrm{i}k_0+l-1) & & \\
\vdots & & & & \\
\hat{y}^{(l)}(\mathrm{i}k_0+1) & & & &
\end{tikzcd}
$$

3.2. Numerical evaluation of $\hat{y}(\mathrm{i}k_0+t)$

We want to study equation (2.14) on the half-line $\{s=t+\mathrm{i}k_0\colon t\in[1, +\infty)\}$. After the change of variables

$$x=\frac{1}{t}=\frac{1}{s-\mathrm{i}k_0}, \qquad t\in[1, +\infty),$$

$$\Phi(x)=\hat{y}\left(\mathrm{i}k_0+\frac{1}{x}\right)\left[\left(\mathrm{i}k_0+\frac{1}{x}\right)^2+k_0^2\right]^{-l},$$

equations (2.14), (2.13*b*) can be written in the form

$$\frac{\mathrm{d}\Phi(x)}{\mathrm{d}x}=-\lambda_0(x+1)^l\frac{[(1+2\mathrm{i}k_0)x+1]^l}{(2\mathrm{i}k_0x+1)^{l+1}}\Phi(\alpha(x))$$

$$-\frac{x^{2l}}{(2\mathrm{i}k_0x+1)^{l+1}}, \qquad x\in(0, 1] \tag{3.1a}$$

$$\Phi(0^+)=0, \tag{3.1b}$$

$$\alpha(x)=\frac{x}{x+1}, \qquad x\in(0, 1]. \tag{3.1c}$$

Since $\alpha(x)=x$ for $x=0$, this is a typical RODE problem to which considerable attention has been devoted in the mathematical literature. In particular Feldstein (1964) has proved that under stuitable conditions Euler's scheme converges uniformly to the unique solution of the problem.

In appendix 2 Feldstein's results are summarised and the customary Euler's scheme is described.

Table 1. Convergence of the numerical approach (A.9), (A.10), (A.11) for the problem (3.1); h is the step size.

	$\lambda = 1{\cdot}5933,\ a = 1{\cdot}5636$					$\lambda = 1{\cdot}3471,\ a = 1{\cdot}1706$			
	h	$\hat{y}(ik_0+1)$	First extrapolation	Second extrapolation		h	$\hat{y}(ik_0+1)$	First extrapolation	Second extrapolation
	2^{-5}	−0·22951+i0·02787				2^{-4}	−0·14568+i0·03403		
	2^{-6}	−0·23113+i0·02839	−0·23275+i0·02892			2^{-5}	−0·15333+i0·03827	−0·16099+i0·04252	
$k = 0{\cdot}1$ $l = 1$	2^{-7}	−0.23190+i0·02864	−0·23267+i0·02889	−0·23264+i0·02888	$k = 0{\cdot}25$ $l = 2$	2^{-6}	−0·15701+i0·04031	−0·16068+i0·04235	−0·16057+i0·04229
	2^{-8}	−0.23227+i0·02876	−0·23265+i0·02888	−0·23264+i0·02888		2^{-7}	−0·15880+i0·04131	−0·16060+i0·04231	−0·16058+i0·04229
	2^{-9}	−0·23246+i0·02882	−0·23265+i0·02888	−0·23264+i0·02888		2^{-8}	−0·15969+i0·04180	−0·16058+i0·04229	−0·16058+i0·04229
	2^{-5}	−0·02078+i0·03094				2^{-4}	−0·01839+i0·02438		
	2^{-6}	−0·02141+i0·03237	−0·02204+i0·03381			2^{-5}	−0·01965+i0·02775	−0·02091+i0·03113	
$k = 1{\cdot}25$ $l = 5$	2^{-7}	−0·02174−i0·03309	−0·02207+i0·03380	−0·02208+i0·03380	$k = 1{\cdot}5$ $l = 6$	2^{-6}	−0·02031+i0·02948	−0·02098+i0·03121	−0·02100+i0·03123
	2^{-8}	−0·02191+i0·03345	−0·02208+i0·03380	−0·02208+i0·03380		2^{-7}	−0·02066+i0·03035	−0·02100+i0·03123	−0·02101+i0·03123
	2^{-9}	−0·02199+i0·03362	−0·02208+i0·03380	−0·02208+i0·03380		2^{-8}	−0·02083+i0·03079	−0·02101+i0·03123	−0·02101+i0·03123

Table 2. Comparison with the numerical integration of Swan (1960a, b). Potential function $V = -\lambda[\exp(-r/a)]r$.

		^3S n–p scattering: $\lambda = 1{\cdot}5933$; $a = 1{\cdot}5636$						^1S n–p scattering: $\lambda = 1{\cdot}34710$; $a = 1{\cdot}1706$					
	$k = k_0/a$	δ_1	δ_2	δ_3	δ_4	δ_5	δ_6	δ_1	δ_2	δ_3	δ_4	δ_5	δ_6
	0·1	0·00667						0·00173					
	0·25	0·07389	0·00592					0·02163	0·00116				
Our	0·5	0·24871	0·05101	0·01253				0·09458	0·01453	0·00258			
results	0·75	0·35270	0·11167	0·04100	0·01530			0·16344	0·04072	0·01148	0·00342		
	1·0	0·39595	0·15978	0·07086	0·03307	0·01591		0·20747	0·06838	0·02495	0·00957	0·00378	
	1·5	0·41073	0·21276	0·11823	0·06837	0·04055	0·02446	0·24495	0·10936	0·05277	0·02657	0·01372	0·0721
	0·1	0·0110						0·0018					
	0·25	0·0894	0·0080					0·0229	0·0012				
Swan	0·5	0·2513	0·0589	0·0178				0·1009	0·0189	0·0026			
(1960a, b)	0·75	0·3548	0·1163	0·0430	0·0247			0·1665	0·0421	0·0132	0·0036		
	1·0	0·3983	0·1627	0·0736	0·0349	0·0187		0·2100	0·0705	0·0262	0·0101	0·0040	
	1·5	0·4123	0·2141	0·1194	0·0693	0·0421	0·0255	0·2357	0·1089	0·0541	0·0273	0·0147	0·0083
Born	0·1	0·0057						0·0016					
approxi-	0·25	0·0602	0·0057					0·0195	0·0011				
mation,	0·5	0·1990	0·0503	0·0123				0·0827	0·0143	0·0026			
Swan	0·75	0·2989	0·1196	0·0389	0·0152			0·1445	0·0420	0·0113	0·0034		
(1960a, b)	1·0	0·3544	0·1818	0·0696	0·0335	0·0158		0·1880	0·0741	0·0245	0·0096	0·0038	
	1·5	0·4147	0·2763	0·1266	0·0700	0·0418	0·3190	0·2383	0·1343	0·0533	0·0275	0·0138	0·0078

It is easy to show that problem (3.1) meets the requirements of the theorem quoted in appendix 2 so that Euler's scheme converges uniformly on [0, 1]. It is a first-order algorithm (that is, the error is proportional to the step size h). However, if Richardson's extrapolation procedure is applied m times the computational scheme becomes of order h^{1+m} (Henrici 1962, Feldstein 1964).

The code YUKAL (which has been run on the IBM 370/158 of the CSATA laboratories, Bari) employs the Euler scheme to evaluate the numerical values of $\hat{y}$. Table 1 exhibits the convergence properties of the scheme. Moreover, the code treats the numerical values of $\hat{y}$ at $\mathrm{i}k_0+1, \ldots, \mathrm{i}k_0+l+1$ according to the procedures of § 3.1 and evaluates c_l, S_l, δ_l.

4. Numerical comparisons

Here we wish to compare our results with the corresponding results that have appeared in the literature. We have found remarkable agreement between our numerical estimates and those obtained in an early treatment (Hulthèn 1944) in which a variational principle is employed for the calculation of the phase shift δ_l. For $l=0$, $k_0=0{\cdot}8$ and: (i) $\lambda_0=1{\cdot}5$; (ii) $\lambda_0=2.1$; Hulthèn obtains: (i) $\delta_0=0{\cdot}83708\ldots$; (ii) $\delta_0=1{\cdot}27515\ldots$; and claims that the error 'probably does not exceed a couple of units in the fifth decimal'. We find the exact results: (i) $\delta_0=0.83708\ldots$; (ii) $\delta_0=1{\cdot}27516\ldots$

Our results are displayed together with estimates based on the numerical integration of the Schrödinger equation in tables 2, 3, 4. As a consequence of partial wave

Table 3. Comparison with the numerical integration of Gerjouy and Saxon (1954). Potential function $V=-\lambda[\exp(-r/a)]/r$; $a=1{\cdot}35\times10^{-13}$ cm; $\lambda a=2{\cdot}365$; $k_0=ka$. The differential cross section is given in units of a^2, the total cross section in units of πa^2.

		Differential cross section		Total cross section	
k_0	Angle	Our results	Gerjouy and Saxon (1954)	Our results	Gerjouy and Saxon (1954)
	0	4·083	3·99		
0·6630	$\pi/2$	2·282	2·28	10·09	10·1
	π	2·292	2·27		
	0	4·795	4·58		
1·048	$\pi/2$	0·7534	0·752	4·540	4·53
	π	0·5105	0·531		
	0	5·140	5·07		
1·406	$\pi/2$	0·3085	0·309	2·645	2·64
	π	0·1506	0·151		
	0	5·255	5·25		
1·624	$\pi/2$	0·1894	0·190	2·015	2·01
	π	0·0796			
	0	5·312	5·31		
1·816	$\pi/2$	0·1272	0·127	1·628	1·63
	π	0·0482	0·048		

Table 4. Comparison with the numerical integration of Mower (1955). Potential function $V=-\lambda[\exp(-r/a)]/r$; $a=\frac{3}{8}a_0$; $\lambda_0=\lambda a=5\cdot84$; $k_0=ka=0\cdot72$. Here a_0 is the first Bohr radius. The differential cross section is given in units of a^2.

	Phase shifts				Differential cross section		
	δ_0	δ_1	δ_2	δ_3	0	$\pi/2$	π
Our results	3·280	0·8844	0·1083	0·0225	2·477	0·00370	1·033
Mower (1955)	3·28	0·888	0·110	0·021	2·41	0·005	1·05

analysis,

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}=|f(\theta)|^2=\left|\frac{1}{2ik}\sum_l[\exp(2i\delta_l)-1](2l+1)P_l(\cos\theta)\right|^2$$

is the differential cross section, where P_l is the Legendre polynomial of degree l. Finally for the total cross section, one has

$$\sigma=\int\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\mathrm{d}\Omega=\frac{4\pi}{k^2}\operatorname{Im}(f(0))$$

where the so called optical theorem has been used.

5. Conclusions

The Laplace transform as a technique of asymptotic analysis has been applied to a specific scattering problem to derive a numerical scheme for the computation of the S matrix.

The authors feel that the main features of the treatment presented here are the following:

(i) Theorems which connect the asymptotic parameters of the transform with the asymptotic parameters of the wavefunction in an exact way are exploited in a computationally convenient form.

(ii) The *convergent* numerical scheme which is employed permits the evaluation of the relevant parameters as precisely as desired.

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Appendix 1. Some Abelian asymptotic theorems

In this appendix we summarise—after some minor adjustments—some results from

Doetsch (1955, in German). Under the assumption that the Laplace transform

$$\hat{f}(s)=\mathscr{L}[f]=\int_0^{+\infty}\exp(-s\xi)f(\xi)\,\mathrm{d}\xi$$

has a finite abscissa of convergence α and that it has a finite number m of singularities on the vertical line $\{\mathrm{Re}(s)=\alpha\}$, we shall connect the asymptotic behaviour of $\hat{f}(s)$ in the neighbourhood of the singularities with the asymptotic behaviour of $f(\xi)$ for $\xi\to+\infty$.

Suppose that $\hat{f}$ admits an analytic continuation on $\{\mathrm{Re}(s)\geqslant\alpha\}$ with the exception of the singular points:

$$s_k=\alpha+\mathrm{i}\Omega_k, \qquad k\in\{1,2,\ldots,m\},$$

where for all k, $\Omega_k\in\mathbb{R}$; $\alpha\in\mathbb{R}$; m is a positive integer; and where α, m are finite. Now let

$$\begin{aligned}
\hat{f}_{1k}(s)&=\sum_{\nu=0}^{n}c_{\nu k}(s-s_k)^{\lambda_{\nu k}},\\
\hat{f}_{2k}(s)&=\ln(s-s_k)\sum_{\nu=0}^{n}c_{\nu k}(s-s_k)^{\nu+\mu},\\
\hat{f}_{3k}(s)&=\ln(s-s_k)\sum_{\nu=0}^{n}c_{\nu k}(s-s_k)^{\lambda_{\nu k}},
\end{aligned} \tag{A.1}$$

where it is assumed that μ is a non-negative integer and where

$$\forall k\in\{1,2,\ldots,m\}:\mathrm{Re}(\lambda_{0k})<\mathrm{Re}(\lambda_{1k})\ldots<\mathrm{Re}\,(\lambda_{nk}),$$
$$\forall(\nu,k)\in\{0,1,2,\ldots,n\}\times\{1,2,\ldots,m\}:\lambda_{\nu k}\notin\{0,1,2,\ldots\}.$$

Moreover, let

$$\begin{aligned}
f_{1k}(\xi)&=\exp(s_k\xi)\sum_{\nu=0}^{n}(c_{\nu k}/\Gamma(-\lambda_{\nu k}))\xi^{-\lambda_{\nu k}-1},\\
f_{2k}(\xi)&=-\exp(s_k\xi)\sum_{\nu=0}^{n}c_{\nu k}(-1)^{\nu+\mu}(\nu+\mu)!\,\xi^{-\nu-\mu-1},\\
f_{3k}(\xi)&=-\exp(s_k\xi)\sum_{\nu=0}^{n}(c_{\nu k}/\Gamma(-\lambda_{\nu k}))\xi^{-\lambda_{\nu k}-1}\left(\ln(\xi)-\frac{\Gamma'(-\lambda_{\nu k})}{\Gamma(-\lambda_{\nu k})}\right).
\end{aligned}$$

Now consider the asymptotic behaviours

$$f(\xi)\sim\sum_{k=1}^{m}f_{jk}(\xi), \qquad \text{for } \xi\to+\infty, \tag{A.2}$$

$$\hat{f}(s)\sim\hat{f}_{jk}(s), \qquad \text{for } s\to s_k,\ \forall k\in\{1,2,\ldots,m\}, \tag{A.3}$$

which are supposed to hold for some $j\in\{1,2,3\}$; theorems 1, 2, 3 to be quoted establish conditions under which (A.2) implies (A.3) or conversely (A.3) implies (A.2).

The theorems are slightly revised versions of Doetsch (1955, *Satz* 1, chap. 4, § 2; *Satz* 1, chap. 7, § 3; *Satz* 2, chap. 7, § 2).

Theorem 1. Let $f: [0, +\infty) \to \mathbb{R}$ be piecewise continuous. For some $j \in \{1, 2, 3\}$ suppose that a parameter $\epsilon > 0$ exists such that

$$f(\xi) = \sum_{k=1}^{m} f_{jk}(\xi) + O(\exp(\alpha - \epsilon)\xi), \qquad \text{for } \xi \to +\infty, \tag{A.4}$$

where $1 \leq m < +\infty$. Then $\hat{f}(s) = \int_0^{+\infty} \exp(-s\xi) f(\xi)\, d\xi$ has abscissa of convergence α. Moreover, the function

$$\hat{g}(s) = \hat{f}(s) - \sum_{k=1}^{m} \hat{f}_{jk}(s) \tag{A.5}$$

admits an analytic continuation on the strip $\{\alpha - \epsilon < \mathrm{Re}(s) \leq \alpha\}$ (with no singularities there).

Conversely we have the following theorem.

Theorem 2. Suppose that:

(a) $f: [0, +\infty) \to \mathbb{R}$ is piecewise continuous, and $\hat{f}(s) = \int_0^{+\infty} \exp(-s\xi) f(\xi)\, d\xi$ has the finite abscissa of convergence α;

(b) for $\omega \in \mathbb{R}$, $\lim_{|\omega| \to +\infty} (\partial/\partial\omega)^R \hat{f}(\alpha + i\omega) = 0$, $\forall R \in \{1, 2, \ldots\}$;

(c) a parameter $\beta > \alpha$ exists such that $\lim_{|\omega| \to +\infty} \hat{f}(\gamma + i\omega) = 0$, $\forall \gamma \in [\alpha, \beta]$, uniformly;

(d) for some $j \in \{1, 2, 3\}$, $\hat{g}(s)$—defined by equation (A.5)—is continuous on $\{\mathrm{Re}(s) \geq \alpha\}$;

(e) The derivatives $(\partial/\partial\omega)^R \hat{g}(\alpha + i\omega)$ exist for all $\omega \in \mathbb{R}$ and for all $R \in \{1, 2, \ldots\}$.

Then

$$f(\xi) = \sum_{k=1}^{m} f_{jk}(\xi) + o(e^{\alpha\xi}\xi^{-\rho}), \qquad \text{for } \xi \to +\infty \tag{A.6}$$

where ρ is any positive parameter.

The basic result of theorem 2 can be presented in a different form: requirements (b) and (c) are omitted, but an analytical continuation for $\hat{f}$ to the left of the abscissa of convergence is performed. Indeed for a given $\psi \in (\frac{1}{2}\pi, \pi)$ let

$$S_k(\psi) = \{s \in \mathbb{C}: \tfrac{1}{2}\pi \leq |\arg(s - s_k)| \leq \psi \text{ and } |s - s_k| > 0\}$$

$$S(\psi) = \bigcap_{k \in \{1, 2, \ldots, m\}} S_k(\psi).$$

Then we have the following theorem.

Theorem 3. Under assumption (a) of theorem 2, suppose that:

(b) a parameter $\psi \in (\frac{1}{2}\pi, \pi)$ exists such that $\hat{f}$ admits an analytical continuation on $S(\psi)$; moreover $\lim_{|s| \to +\infty} \hat{f}(s) = 0$ uniformly with respect to $\arg(s)$ with $s \in S(\psi)$;

(c) for some $j \in \{1, 2, 3\}$ and for each $k \in \{1, 2, \ldots, m\}$, equation (A.3) holds uniformly with respect to $\arg(s - s_k)$ with $0 \leq |\arg(s - s_k)| \leq \psi$.

Then (A.2) holds.

On comparing the different forms which the asymptotic results (A.2), (A.3) take in theorems 1, 2, 3 we observe:

(i) Result (A.6) of theorem 2 provides a sharp estimate of the asymptotic behaviour of the error $e(\xi)=f(\xi)-\Sigma_{k=1}^{m} f_{jk}(\xi)$ whereas theorem 3 provides limited information on the error's properties.

(ii) Assumption (*d*) of theorem 2 is strictly connected to assumption (*c*) of theorem 3; hence it is connected to the asymptotic law (A.3). It should be noted that in (*c*) of theorem 3 equation (A.3) is required to hold for $|\arg(s-s_k)|\leq\psi$ with $\psi>\frac{1}{2}\pi$ whereas (*d*) of theorem 2 corresponds to the case $\psi=\frac{1}{2}\pi$. However in theorem 2 further requirements are imposed on the 'error' $\hat{g}(s)$.

Appendix 2. The Euler algorithm for a retarded ordinary differential equation

This appendix summarises some pertinent results from Feldstein's dissertation (1964) in which the RODE initial value problem is considered:

$$\begin{aligned} &\frac{\mathrm{d}}{\mathrm{d}x} y(x)=f(x, y(x), y(\alpha(x))), && 0\leq x\leq 1, \\ &y(0)=y_0\in\mathbb{R}, \qquad 0\leq\alpha(x)\leq x, && 0\leq x\leq 1. \end{aligned} \tag{A.7}$$

Here α is an assigned function. Let

$$\begin{aligned} &h=1/N \quad (N \text{ positive integer}), \\ &x_n=nh \\ &q(n)=[\alpha(x_n)/h] \qquad r(n)=\alpha(x_n)/h-q(n) \end{aligned} \tag{A.8}$$

where $[\eta]$ denotes the integer part of η. Then Feldstein's 'customary Euler algorithm' is

$$z_0=y(0) \qquad z_n=y_{q(n)}+hr(n)f_{q(n)} \tag{A.9}$$

$$f_n=f(x_n, y_n, z_n) \tag{A.10}$$

$$y_0=y(0) \qquad y_{n+1}=y_n+hf_n. \tag{A.11}$$

The main result is given in the following theorem (Feldstein 1964, theorem 1.1):

Theorem. Let $\alpha\in C^p([0,1],\mathbb{R})$, $f\in C^p([0,1]\times\mathbb{R}\times\mathbb{R},\mathbb{R})$ where p is a positive integer. Moreover, suppose that f obeys the global Lipschitz condition $|f(x,y,z)-f(x,\bar{y},\bar{z})|<L(|y-\bar{y}|+|z-\bar{z}|)$, $\forall(x,y,z,\bar{y},\bar{z})\in[0,1]\times\mathbb{R}^4$, where $0<L<+\infty$. Then the RODE problem (A.7) admits an unique solution y of class $C^{p+1}([0,1],\mathbb{R})$. Moreover, the customary Euler algorithm (A.8) to (A.11) converges uniformly to y on $[0,1]$ for $N\to+\infty$.

We wish to observe that this result can be easily generalised to the case in which y, f are complex valued.

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