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1980 J. Phys. A: Math. Gen. 13 3287

(http://iopscience.iop.org/0305-4470/13/10/024)

J. Phys. A: Math. Gen. **13** (1980) 3287–3301. Printed in Great Britain

Evaluation of the S matrix for a class of potentials

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Received 6 March 1980

Abstract. As an extension of a previous treatment, the S-matrix problem is studied for the radial potential $V(r) = -(\mu + \lambda/r)\exp(-r)$. The Schrödinger equation is Laplace transformed. Then results on the asymptotics of the Laplace transformation are used to express the S-matrix element S_l as a linear combination of the values of the transformed function and of its first $l+1$ derivatives at one point in the complex plane. By a change of variables, the evaluation of S_l and of the phase shift δ_l is then reduced to the numerical solution of a non-singular neutral functional differential equation (on a finite interval) followed by a finite recursive procedure. A convergent numerical scheme is implemented. Comparisons with literature results are performed.

1. Introduction

In this paper we consider the S-matrix problem for the radial Schrödinger equation

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

with $k>0$ and $l \in \mathbb{N} = \{0, 1, 2, \ldots\}$, under the assumption that for all $r>0$ the potential function V obeys

$$V(r) = -(\mu + \lambda/r)\,\mathrm{e}^{-r/a} \qquad (\text{with } a>0;\ \lambda, \mu \in \mathbb{R};\ |\lambda|+|\mu|>0). \tag{1.2}$$

This class of potentials is important since it includes a number of cases which appear frequently in the literature. Indeed, for $\mu = 0$ and $\lambda \neq 0$, equation (1.2) yields the Yukawa potential; for $\mu \neq 0$ and $\lambda = 0$, it yields the exponential potential; for $\lambda \neq 0$ and $\mu \neq 0$, it yields the static potential approximation for the three-body problem.

Now, it is clear that for all potentials of class (1.2) one has

$$\begin{aligned} &V(.) \in \mathscr{C}((0, +\infty), \mathbb{R}), \\ &\int_0^1 r|V(r)|\,\mathrm{d}r < +\infty, \qquad \int_1^{+\infty} |V(r)|\,\mathrm{d}r < +\infty. \end{aligned} \tag{1.3}$$

Then, employing a well established result (see, e.g., Reid and Simon 1979, theorem XI 53, Newton 1966 § 11.1 and 12.1), we can claim that there is a unique real-valued function $u(r)$ which obeys equation (1.1), subject to (1.2), for all $r \in (0, +\infty)$ and which

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satisfies the constraints

$$\sup\{|u(r)|: r \in (0, +\infty)\} < +\infty, \qquad \lim_{r \to 0^+} r^{-(l+1)} u(r) = v_0 \in \mathbb{R} - \{0\}. \quad (1.4)$$

The function u has the asymptotic property

$$u(r) = v_0 A \sin(kr - \tfrac{1}{2} l\pi + \delta_l) + o(1), \qquad \text{for } r \to +\infty,$$

for some $\delta_l \in \mathbb{R}$ and for some $A \in \mathbb{R} - \{0\}$. In the literature, δ_l is known as phase shift, whereas $S_l = \exp(2i\delta_l)$ is known as the lth element of the S matrix. One can show that for each assignment of $k > 0$ and $l \in \mathbb{N}$, and for each choice of the potential function V satisfying the requirements (1.3), $S_l \in \mathbb{R}$ is unique, whereas $\delta_l \in \mathbb{R}$ is unique *modulo* π. Also, S_l is a functional of V and is a function of k and l; it is independent of v_0.

In a previous paper (Paiano and Paveri-Fontana 1978 (see also 1979), hereafter referred to as I), we have presented a convergent numerical procedure for the computation of the S-matrix element S_l for the Yukawa potential problem. In this paper we extend our previous treatment to allow for all potentials of class (1.2). As in I, the procedure hinges on some Abelian results which connect the behaviour of $y(\xi) = \xi^{-(l+1)} u(a\xi)$ as $\xi \to +\infty$ to the behaviour of its Laplace transform,

$$\hat{y}(s) = \mathscr{L}[y(\xi)] = \int_0^{+\infty} \exp(-s\xi) y(\xi)\, d\xi, \quad (1.5)$$

in the neighbourhood of its rightmost singularities in the complex s plane. In I as well as here, the estimation procedure for S_l does not involve a complex plane integration. On the contrary, after Laplace transforming the Schrödinger equation (1.1) into a difference–differential equation and after performing a change of variables, we show that the evaluation of S_l follows—with the help of a recursive procedure—from the solution of a pertinent initial-value problem for a non-singular functional equation on a finite interval. For the solution of the initial-value problem we make use of a convergent numerical procedure. In this paper we shall rely on the results presented in I and we shall omit some mathematical details. We would like to remark, incidentally, that the lengthy treatment in § 2 of I could have been slightly streamlined by the omission of the uniqueness theorem (proposition 2 there); indeed, the uniqueness of results follows in I from the direct application of the basic theorem of appendix 2 to the retarded ordinary differential problem (3.1). We would also like to mention that Laplace transform procedures for the S-matrix problem have been developed by other authors (Almström 1969, 1970, Englefield 1968, 1974) in research work of analytical slant. Partial overlap is acknowledged. See also Leasure and Bowman (1978).

We mentioned that our object is to establish a reliable convergent procedure (an 'exact' procedure) for the computation of S_l and δ_l. The literature on this subject is extensive. Our survey in I was scant. Here, in order to illustrate the motivation of our work and its position with respect to the published literature, we would like to present some further literature information: the survey will be brief and, of course, no completeness is claimed. In the literature, distinct computational approaches for the phase shift problem have been developed, starting from three alternative (but equivalent) formulations of the problem: (i) the (linear second-order) radial Schrödinger equation formulation, equations (1.1) and (1.4); (ii) its (nonlinear first-order) Riccati counterpart, and the related variable phase formulation; (iii) the Fredholm integral equation formulation (there are several versions, all related to the Lippman–Schwinger equation). For the actual evaluation of S_l and δ_l based on one of

the three formulations, several philosophies have been implemented. Here we choose—somewhat arbitrarily—to classify them as: (a) analytical; (b) approximate; (c) numerical. *Analytical* results have been obtained only for a limited number of cases. For instance, in the early work of Bethe and Bacher (1936) one finds the solution for the S-wave exponential potential case ($\lambda = 0$, $\mu \neq 0$, $l = 0$); recently Bühring (1977) has presented an expression for S_l in the Yukawa case ($\lambda \neq 0$, $\mu = 0$, for all $l \in \{0, 1, 2, \ldots\}$) in terms of a convergent double series of hypergeometric functions. *Approximate* methods include the well known Born approximation (see, e.g., Newton 1966, Taylor 1972), the Fredholm and the Padé approximant approaches (Reinhardt and Szabo 1970, Moisewitsch 1970, Moisewitsch and O'Brien 1970), and finally the variational approach (see, e.g., Mott and Massey 1965 for a review of early results; see also Rudge 1973 for more recent results, and Darewych and Pooran 1978 for error estimates). The main competitors of our method are the procedures involving the direct *numerical* solution of the problem. In the literature one finds several studies of the phase shift problem by means of a numerical treatment of the Schrödinger equation. The main difficulty is due to the fact that one is forced to solve numerically the Schrödinger equation on a finite interval $(0, \tilde{r})$ with some step-size h; then, to estimate $\tilde{\delta}_l$ by some matching procedure at $\tilde{r}$; finally, to study the behaviour of $\tilde{\delta}_l$ under the double limit $h \to 0^+$, $\tilde{r} \to +\infty$. In the literature the numerical treatment of the Schrödinger equation has been performed using, among others, the Numerov method, the Runge–Kutta method and also the DeVogelaere method (see e.g., Allison 1970, Kermode and McKerrell 1975, Stern 1977, Coleman and Mohamed 1979). In so far as we know, no proof of convergence of $\tilde{\delta}_l$ to the exact value has been established. From a more empirical standpoint, convergence difficulties for some cases have been found, for instance by Stern (1977 p 61); see also table 5 of this paper. The numerical treatment according to the variable phase—or the Riccati—formulation (Calogero 1967, Kermode 1968, Klozenberg 1974) also involves the numerical solution of a differential equation on a finite interval $(0, \tilde{r})$ with some step-size h, followed by a limiting process as $h \to 0^+$ and $\tilde{r} \to +\infty$. However, no matching is required at $\tilde{r}$; in addition, error bounds for finite $\tilde{r}$ can be established (one can use, for instance, equation (3.13) of Calogero 1963). Good convergence patterns have been exhibited in the literature (Calogero 1967). Table 6 of this paper compares our results with those obtained by Common (1979) employing Klozenberg's (1974) PHASE code for the variable phase equation. Numerical work on the Fredholm integral version of the phase shift problem has been performed, for instance, by Holt and Santoso (1972) and by Stern (1977, 1978). Proofs of convergence have not been given. In practice, difficulties originate here from the fact that one has to invert a matrix whose dimensions grow as the discretisation parameter shrinks. Finally, our method reduces the computation of S_l and δ_l to the numerical solution of a non-singular linear functional differential equation on a finite interval, followed by a finite recursive procedure. Convergence is established.

This paper is organised as follows. In § 2 the analytical results of § 2 of I—which concerned the Yukawa potential case ($\mu = 0$, $\lambda \neq 0$)—are generalised to the class of potentials (1.2). It is shown that the Laplace transformed function $\hat{y}$ obeys a difference–differential equation and that $S_l = -c_l/\bar{c}_l$; here a bar denotes complex conjugation and c_l can be expressed as a linear combination of $\hat{y}(s)$ and its first $(l+1)$ derivatives (its first l derivatives in the Yukawa case) at $s = \mathrm{i}ak + 1$. The mathematical background has been established in appendix 1 of I, following Doetsch (1955). Section 3 of this paper corresponds to § 3 of I. For $\mu \neq 0$ some complications arise and a computational treatment which is slightly more involved than the one described in I becomes

necessary. In I a recursive procedure was applied to the numerical solution of an initial-value problem—equations (3.1) there—for a *retarded* (or delayed) differential equation. In the present paper a different recursive procedure is applied to the numerical solution of an initial-value problem—equation (3.11)—for a *neutral* functional differential equation†. The new procedure can be employed in the Yukawa case; however, even in this case it is not completely coincident with the procedure in I. This fact provides a convenient procedure for checking the reliability of the numerical implementation of the two procedures (table 3). In § 4 results are reported on the computation of the phase shift δ_l in a number of cases. Whereas in I we have employed Feldstein's 'customary Euler algorithm' (Feldstein 1964, Cryer 1972 § 1.2.1), in this paper we employ a trapezoidal scheme both for the *retarded* problem of I and for the *neutral* problem found here. An increase in the speed of convergence is found. The trapezoidal scheme is described in the Appendix.

2. The analytical treatment

In this section we shall follow closely § 2 of I. Most details and proofs will be omitted.

After the change of variables $\xi = r/a$, $k_0 = ka$, $\lambda_0 = \lambda a$, $\mu_0 = \mu a^2$, $y_0 = v_0 a^{l+1}$ and $y = \xi^{-(l+1)}u$, equations (1.1), (1.2) and (1.4) yield

$$\left(\xi\frac{d^2}{d\xi^2} + 2(l+1)\frac{d}{d\xi} + (k_0^2\xi + \lambda_0 e^{-\xi} + \mu_0\xi e^{-\xi})\right)y(\xi) = 0, \qquad \xi > 0, \tag{2.1a}$$

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

$$y(0^+) = y_0. \tag{2.1c}$$

Here k_0, l, y_0, λ_0, μ_0 are assigned, subject to the requirements

$$k_0 > 0, \qquad l \in \mathbb{N}, \qquad y_0, \lambda_0, \mu_0 \in \mathbb{R}, \qquad |\lambda_0| + |\mu_0| > 0, \qquad y_0 \neq 0.$$

With reference to the results quoted in the Introduction, we know that problem (2.1) admits a unique solution $y(\xi)$, and that in $[0, \pi) \times (\mathbb{R} - \{0\})$ there is a unique pair (δ_l, A) such that

$$y(\xi) = y_0 A \xi^{-(l+1)} \sin(k_0\xi - \tfrac{1}{2}l\pi + \delta_l) + o(1), \qquad \text{for } \xi \to +\infty. \tag{2.2}$$

One can also show that $y \in \mathscr{C}^\infty((0, +\infty), \mathbb{R})$.

On account of equations (2.1) and (2.2), we can claim that the Laplace integral (1.5) converges on the half-plane $\{s \in \mathbb{C}: \mathrm{Re}(s) > 0\}$ to an analytic function $\hat{y}$, which obeys the equations

$$\frac{d}{ds}\frac{\hat{y}(s)}{(s^2 + k_0^2)^{l+1}} = \frac{\lambda_0\hat{y}(s+1) - \mu_0(d/ds)\hat{y}(s+1) - (2l+1)y_0}{(s^2 + k_0^2)^{l+1}}, \qquad \mathrm{Re}(s) > 0. \tag{2.3}$$

Now set

$$\theta(s) = \frac{\lambda_0\hat{y}(s+1) - \mu_0(d/ds)\hat{y}(s+1) - (2l+1)y_0}{(s^2 + k_0^2)^{l+1}}. \tag{2.4}$$

† For a classification of functional differential equations with retarded arguments (delays) see, e.g., El'sgol'ts and Norkin (1973), Hale (1977).

Then, on account of the analyticity of $\hat{y}$ for $\mathrm{Re}(s)>0$, of equation (2.3) and of definition (2.4), we have the Laurent expansions

$$\theta(s)=\sum_{R=0}^{+\infty} c_R(s-\mathrm{i}k_0)^{R-(l+1)}, \qquad \text{for } s\in C_+=\{s\in\mathbb{C}: |s-\mathrm{i}k_0|<b\}; \tag{2.5a}$$

$$\frac{\mathrm{d}}{\mathrm{d}s}\frac{\hat{y}(s)}{(s^2+k_0^2)^l}=\sum_{R=0}^{\infty} c_R(s-\mathrm{i}k_0)^{R-(l+1)}, \qquad \text{for } s\in W_+=C_+\cap\{s\in\mathbb{C}: \mathrm{Re}(s)>0\}, \tag{2.5b}$$

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

$$c_R=\frac{1}{R!}\lim_{s\to \mathrm{i}k_0}\left(\frac{\mathrm{d}}{\mathrm{d}s}\right)^R \frac{\lambda_0\hat{y}(s+1)-\mu_0(\mathrm{d}/\mathrm{d}s)\hat{y}(s+1)-(2l+1)y_0}{(s^2+k_0^2)^{l+1}}, \qquad R\in\mathbb{N}. \tag{2.6}$$

Direct term-by-term integration of equation (2.5*b*) yields

$$\hat{y}(s)=(s+\mathrm{i}k_0)^l\sum_{R=0}^{+\infty} w_R(s-\mathrm{i}k_0)^R+c_l\ln(s-\mathrm{i}k_0)\sum_{\nu=0}^{l}\binom{l}{\nu}(2\mathrm{i}k_0)^{l-\nu}(s-\mathrm{i}k_0)^{l+\nu}, \qquad s\in W_+, \tag{2.7}$$

where $w_R=c_R/(R-l)$ for $R\neq l$, and where w_l is some appropriate complex number. A similar result holds in the vicinity of $-\mathrm{i}k_0$ on account of the reflection principle $\hat{y}(\bar{s})=\overline{\hat{y}(s)}$. Expansion (2.7) suggests that the points $+\mathrm{i}k_0$ and $-\mathrm{i}k_0$ are branch points for the function $\hat{y}$. If one introduces in the complex plane the cuts $\Gamma_+=\{s\in\mathbb{C}: \mathrm{Im}(s)=+k_0 \text{ and } \mathrm{Re}(s)\leqslant 0\}$ and $\Gamma_-=\{s\in\mathbb{C}: \mathrm{Im}(s)=-k_0 \text{ and } \mathrm{Re}(s)\leqslant 0\}$, one finds that $\hat{y}$ can be continued analytically on $\mathbb{C}-(\Gamma_+\cup\Gamma_-)$. For details, reference should be made to *proposition* 4 and *figure* 1 of I.

In expansion (2.7) there is a regular part as well as a singular (logarithmic) part. Restricting our attention to the leading terms of the singular contribution, we have

$$\hat{y}(s)=\hat{f}_+(s)(1+\mathrm{O}(s^{-1})), \qquad \text{for } s\to+\mathrm{i}k_0,$$
$$\hat{y}(s)=\hat{f}_-(s)(1+\mathrm{O}(s^{-1})), \qquad \text{for } s\to-\mathrm{i}k_0,$$

where

$$\hat{f}_+(s)=c_l(2\mathrm{i}k_0)^l(s-\mathrm{i}k_0)^l\ln(s-\mathrm{i}k_0), \qquad \hat{f}_-(s)=\overline{\hat{f}_+(\bar{s})}.$$

One can show that the assumptions of theorem 3 of appendix 1 of I are met. Hence

$$\begin{aligned} y(\xi)&=\mathscr{L}^{-1}[\hat{f}_+(s)+\hat{f}_-(s)]+\mathrm{o}(\xi^{-(l+1)})\\ &=2|c_l|l!\,\xi^{-(l+1)}(-2k_0)^l\sin(k_0\xi+\arg(c_l)-\tfrac{1}{2}(l+1)\pi)+\mathrm{O}(\xi^{-(l+1)}),\\ &\quad \text{for } \xi\to+\infty. \end{aligned} \tag{2.8}$$

Comparison of (2.8) with (2.2) yields

$$\delta_l=\arg(c_l)-\tfrac{1}{2}\pi \text{ (modulo } \pi), \tag{2.9a}$$

and also

$$S_l=-c_l/\bar{c}_l, \tag{2.9b}$$

where, on account of equation (2.6),

$$c_l = -(2ik_0)^{-(2l+1)}(2l+1)y_0\binom{-l-1}{l} + \sum_{R=0}^{l}\frac{(2ik_0)^{-(2l+1-R)}}{R!}\binom{-l-1}{-R}\left[\lambda_0\left(\frac{d}{ds}\right)^R\hat{y}(s)-\mu_0\left(\frac{d}{ds}\right)^{R+1}\hat{y}(s)\right]_{s=ik_0+1}. \tag{2.10}$$

It is then clear that we can evaluate S_l if we know the value of $\hat{y}$ and of its first $(l+1)$ derivatives (its first l derivatives in the Yukawa potential case, $\mu_0 = 0$) at the non-singular point ik_0+1.

As a final remark, we note that, as expected, for $\mu_0 = 0$ all equations of this section reduce to their counterparts in I, provided one sets $y_0 = -1/(2l+1)$.

3. The computational procedure

3.1. Preliminary remarks

Restricting our attention to the behaviour of $\hat{y}$ on the half-line $\{s \in \mathbb{C}: \mathrm{Im}(s) = +k_0 \text{ and } \mathrm{Re}(s) \geqslant 1\}$, we introduce the notation

$$z(t) = \hat{y}(t+ik_0), \tag{3.1a}$$

$$D^R z(t) = \begin{cases} 0, & R = -1, \\ z(t), & R = 0, \\ (d/dt)^R z(t), & R = 1, 2, 3, \ldots, \end{cases} \tag{3.1b}$$

for $t \in [1, +\infty)$. On account of equations (2.9), we are specifically interested in establishing an algorithm for the evaluation of $D^R z$ at $t = 1$ for $R \in \{0, 1, 2, \ldots, l+1\}$ (for $R \in \{0, 1, 2, \ldots, l\}$ in the Yukawa case).

We know that $z \in \mathscr{C}^\infty([1, +\infty), \mathbb{C})$. Moreover, equations (2.1c) and (2.3) yield, for $R \in \mathbb{N}$,

$$(t^2+2ik_0t)D^{R+1}z(t) - 2(t+ik_0)(l-R)D^R z(t) - R(2l+1-R)D^{R-1}z(t) = \lambda_0 D^R z(t+1) - \mu_0 D^{R+1}z(t+1) - (2l+1)\delta_{R0}y_0, \qquad t \geqslant 1, \tag{3.2}$$

$$D^R z(t) \sim (-1)^R y_0 R!\,(t+ik_0)^{-(R+1)}, \qquad \text{for } t \to +\infty, \tag{3.3}$$

where $\delta_{R0} = 1$ for $R = 0$ and $\delta_{R0} = 0$ for $R \neq 0$.

We can make use of equations (3.2) in two ways.

(i) We can employ them together with the boundary conditions (3.3) to generate differential problems (to be solved numerically).

(ii) We can use them as links connecting the derivatives of z at some point $t \in [1, +\infty)$ to those at $t+1$ (to be used recursively).

In so far as point of view (i) is concerned, the most interesting cases correspond to those values of R for which equations (3.2) establish a *first-order* functional differential equation for $D^R z$. This occurs only for $R = 0$ and for $R = 2l+1$. In the case $R = 0$,

equations (3.2), (3.3) yield

$$\frac{\mathrm{d}}{\mathrm{d}t}z(t)=\frac{1}{t^2+2\mathrm{i}k_0t}\left(2l(t+\mathrm{i}k_0)z(t)-\mu_0\frac{\mathrm{d}}{\mathrm{d}t}z(t+1)+\lambda_0 z(t+1)-(2l+1)y_0\right),$$

$$t\in[1,+\infty), \tag{3.4a}$$

$$z(t)\sim -y_0/(t+\mathrm{i}k_0), \qquad \text{for } t\to+\infty. \tag{3.4b}$$

For $R=2l+1$, setting

$$f(t)=\frac{-1}{(2l+1)!y_0}D^{2l+1}z(t), \qquad t\in[1,+\infty), \tag{3.5}$$

in equations (3.2)–(3.3), we have

$$\frac{\mathrm{d}}{\mathrm{d}t}f(t)=\frac{1}{t^2+2\mathrm{i}k_0t}\left(-2(l+1)(t+\mathrm{i}k_0)f(t)-\mu_0\frac{\mathrm{d}}{\mathrm{d}t}f(t+1)+\lambda_0 f(t+1)\right), \qquad t\in[1,+\infty), \tag{3.6a}$$

$$f(t)\sim(t+\mathrm{i}k_0)^{-2l-2}, \qquad \text{for } t\to+\infty. \tag{3.6b}$$

In so far as point of view (ii) is concerned, the following *remark* is of importance: suppose that for some $\bar{t}\geqslant 1$ and some $L\in\{1,2,3,\ldots\}$, the values of $D^{L-1}z$ and D^Lz are known at $\bar{t}$ and $\bar{t}+1$. Then, setting $R=L$ in equation (3.2) one can proceed to evaluate $D^{L+1}z(\bar{t})$ if and only if $\mu_0=0$ (with $\lambda_0\neq 0$). On the other hand, setting $R=L-1$ in equation (3.2), it is possible to evaluate $D^{L-2}z(\bar{t})$ for all λ_0, $\mu_0\in\mathbb{R}$ (with $|\lambda_0|+|\mu_0|>0$).

This *remark* is the basis for the two distinct treatments described below.

3.1.1. The Yukawa potential case ($\mu_0=0$ *and* $\lambda_0\neq 0$). Suppose that a numerical scheme has been established for problem (3.4). Then, we can proceed to estimate numerically the values of $z(t)$ for $t\in\{1,2,\ldots,l+1\}$. Consistently with the above *remark*, we can now proceed to use recursively the equations (3.2) with $\mu_0=0$. Firstly, setting $R=0$, we evaluate $Dz(t)$ for $t\in\{1,2,\ldots,l\}$; next, we set $R=1$ and evaluate $D^2z(t)$ for $t\in\{1,2,\ldots,l-1\}$; then we set $R=2$ and evaluate $D^3z(t)$ for $t\in\{1,2,\ldots,l-2\}$. We repeat the procedure up to the evaluation of $D^lz(1)$. Now, with the help of equations (3.1), the values of $z(1)$, $Dz(1)$, $D^2z(1),\ldots,D^lz(1)$ can be inserted in equations (2.9) and (2.10) to yield S_l and δ_l. This approach was taken in I: the diagram in § 3.1 of I illustrates the recursive scheme.

3.1.2. The general case. As discussed earlier, when $\mu_0\neq 0$ we can *not* follow the approach in § 3.1.1: the knowledge of the values of $z(t)$ and $Dz(t)$ for $t\in\{1,2,\ldots,l+1\}$ can *not* be used for the evaluation of D^2z for $t\in\{1,2,\ldots,l\}$. We must proceed 'backwards' using the information on the values of $D^Rz(t)$ and $D^{R+1}z(t)$ at $t=1,2,\ldots,L+1$—for some R and some L in $\{1,2,\ldots\}$—to evaluate $D^{R-1}z(t)$ at $t=1,2,\ldots,L$. In the project described here, we proceed as follows. After a change of variables, we solve numerically problem (3.6) and then we employ a numerical scheme for the integral in

$$D^{2l}z(t)=(2l+1)!\,y_0\int_t^{+\infty}f(t')\,\mathrm{d}t'. \tag{3.7}$$

At this point we are in a position to evaluate $D^{2l}z(t)$ and $D^{2l+1}z(t)$ for $t\in$

$\{1, 2, \ldots, 2l+1\}$. We can then employ recursively the equations (3.2) to evaluate first $D^{2l-1}z(t)$ for $t \in \{1, 2, \ldots, 2l\}$, then $D^{2l-2}z(t)$ for $t \in \{1, 2, \ldots, 2l-1\}$, ..., finally $z(t)$ at $t = 1$. The values of $D^L z(1) = D^L \hat{y}(1 + ik_0)$ for $L \in \{0, 1, 2, \ldots, l+1\}$ can then be inserted in equations (2.9) and (2.10) to yield the values of S_l and δ_l.

In the following subsection we shall discuss the numerical treatment of problems (3.4) and (3.6). Here, as a final remark, we would like to point out that in the actual implementation of § 3.1.2—namely, in the 'backward' use of the recursive procedure—in order to avoid underflow and overflow difficulties it is convenient to make use of the recursive equations (3.3) in a new form; this is obtained by rewriting the equations (3.3) in terms of

$$g^R(t) = ((-1)^R / R!\, y_0)(t + ik_0)^{R+1} D^R z(t), \tag{3.8}$$

rather than in terms of $D^R z$.

3.2. The numerical treatment of problems (3.6) and (3.4)

After the change of variables

$$x = 1/t, \tag{3.9a}$$

$$\psi(x) = ((1 + 2ik_0 x)/x^2)^{l+1} f(1/x), \tag{3.9b}$$

$$\eta(x) = g^{2l}(1/x), \tag{3.9c}$$

and after setting

$$\alpha(x) = x/(x+1), \tag{3.10}$$

problem (3.6) can be written as

$$\frac{\mathrm{d}}{\mathrm{d}x}\psi(x) = -\frac{(1+2ik_0x)^l}{(1+2x(1+ik_0)+x^2(1+2ik_0))^{l+1}} \times \left(\lambda_0 + 2\mu_0(l+1)\frac{(1+x(1+ik_0))x}{1+2x(1+ik_0)+x^2(1+2ik_0)}\psi(\alpha(x)) - \mu_0\frac{x^2}{(1+x)^2}\frac{\mathrm{d}\psi}{\mathrm{d}x}(\alpha(x))\right), \qquad x \in (0, 1], \tag{3.11a}$$

$$\psi(0^+) = 1, \tag{3.11b}$$

where $\mathrm{d}\psi(\alpha(x))/\mathrm{d}x$ stands for $\mathrm{d}\psi(y)/\mathrm{d}y$ evaluated at $y = \alpha(x)$. Making use of (3.9) and (3.10), equation (3.7) yields

$$\eta(x) = \frac{(1+ik_0x)^{2l+1}}{x^{2l+1}} \int_0^x \frac{(2l+1)t^{2l}\psi(t)}{(1+2ik_0t)^{l+1}}\,\mathrm{d}t. \tag{3.12}$$

Problem (3.11) is a non-singular initial-value problem for a neutral equation (see El'sgol'ts and Norkin 1973, or Hale 1977) on a finite interval. It belongs to the class of problems treated in the Appendix. Hence, it admits one and only one solution $\psi \in \mathscr{C}^1([0, 1], \mathbb{C})$. For the numerical treatment, we divide the x-interval $[0, 1]$ in N subintervals of length $h = 1/N$; then we apply the trapezoidal scheme discussed in the Appendix. Piecewise linear interpolation yields $\psi(x)$ for all $x \in [0, 1]$ with an error which is $O(h^2)$ uniformly. We can then turn to equation (3.12). The integral of the RHS is non-singular. On account of the discussion in § 3.1 and of equation (3.9*a*), we are

interested only in the values of $\eta(x)$ for $x \in \{x_1, x_2, \ldots, x_{2l+1}\}$, where $x_k = 1/k$. Now let q_k be the maximum integer such that $hq_k \leqslant 1/k$. To evaluate $\eta(x_k)$ we proceed as follows. We partition the $(0, x_k)$ interval in q_k subintervals of length h—namely, the intervals $(0, h)$, $(h, 2h)$, ..., $((q_k - 1)h, q_k h)$—and in one subinterval of length smaller than h, that is $(q_k h, x_k)$. Then we carry on the numerical evaluation of the integral on the RHS of (3.12), making use of the standard trapezoidal scheme and of the linearly extrapolated expression for ψ. Repeating the procedure we can evaluate $\eta(x_k)$ for all $k \in \{1, \ldots, 2l+1\}$, with error $O(h^2)$ uniformly. Remembering equations (3.5), (3.8) and (3.9), we can now follow § 3.1.2. The 'backward' use of the recursive equations (3.2) permits, with the help of equations (2.9), (2.10) and (3.1), the evaluation of S_l. If we disregard round-off errors, we can claim that the (finite) recursive procedure is exact. Hence we can claim that in the estimate of S_l the error is $O(h^2)$. Applying Richardson's extrapolation we obtain the value of S_l with error $O(h^3)$.

The procedure described above applies to all cases of potentials V obeying equations (1.2) with $\lambda, \mu \in \mathbb{R}$, $|\lambda| + |\mu| \neq 0$. As discussed in § 3.1 of this paper, in the Yukawa case ($\mu = 0$) one can employ equations (3.4) rather than equations (3.6): for this case the counterparts of equations (3.9), (3.10) and (3.11) are given in I. In I the resulting retarded (*not* neutral) initial-value problem was solved numerically, employing Feldstein's 'customary Euler algorithm' (1964). The 'forward' recursive procedure described in § 3.1.1 in the present paper was then implemented, yielding S_l with error $O(h)$†. The results were Richardson extrapolated. Alternatively, the trapezoidal scheme described in the Appendix of the present paper can be applied, followed by the 'forward' recursive procedure. In this case S_l is obtained with error $O(h^2)$. Richardson extrapolation can be performed.

4. Numerical results and comparisons

All the computations were carried out on the IBM 370/158 managed in Bari, Italy by the CSATA laboratories. Tables 1 and 2 illustrate, for specific examples, the rate of convergence for the procedure based on the trapezoidal treatment of equations (3.11) and (3.12), followed by the backward recursive procedure (§ 3.1.2). In table 1 numerical estimates of $\hat{y}(ik_0 + 1) = z(1)$ are tabulated for decreasing values of the step-size h and for given values of λ_0, μ_0, k_0 and l. In table 2 the convergence of the numerical estimate of δ_l as $h \to 0^+$ is illustrated.

Table 3 illustrates the convergence of the numerical estimate of the phase shift δ_l as $h \to 0^+$ for a Yukawa potential problem ($\mu_0 = 0$). For assigned values of λ_0 and l, the first column refers to the numerical solution of equation (3.1) of I by the 'customary Euler algorithm', followed by the forward recursive scheme (§ 3.1.1); the second column refers to the numerical solution of (3.1) of I by the trapezoidal method, also followed by the forward recursive scheme; the third column refers to the numerical treatment of equations (3.10) and (3.12) of this paper by the trapezoidal method, followed by the backward recursive scheme (§ 3.1.2). All results have been Richardson extrapolated once.

As in tables 1 and 2, our results in tables 4 and 5 refer to the trapezoidal treatment of equations (3.10) and (3.12) followed by the backward recursive procedure (§ 3.1.2), and by one Richardson extrapolation. The object of table 4 is to illustrate the accuracy

† In I at page 1709, line 3, one should read '... the error is *roughly* proportional to the step-size h ...'.

of our computations. An S-wave exponential potential problem ($l=0$, $\lambda_0=0$) is treated for which the phase shift δ_0 can be estimated directly from Bessel function theory. Table 5 compares our procedure for the evaluation of δ_l with a numerical procedure (Coleman and Mohamed 1979) which involves the solution of the radial Schrödinger equation on an interval followed by a matching procedure at $\tilde{r}$. The convergence of the two procedures is exhibited in the table (as $h\to 0^+$ in our case, as $\tilde{r}\to+\infty$ for the results of Coleman and Mohamed). The discrepancy in some of the

Table 1. Convergence of the numerical estimate of $\hat{y}(ik_0+1)$. Equations (3.11) and (3.12) are treated according to the trapezoidal scheme. The backward recursive procedure (§ 3.1.2) is implemented. h is the step size. The results in the second column are obtained by Richardson extrapolation of the results in the first column. (*a*) $k_0=0{\cdot}5$, $l=5$; (*b*) $k_0=1{\cdot}5$, $l=3$.

	$\lambda_0=1{\cdot}0$; $\mu_0=0{\cdot}5$	
h	Computed values of $\hat{y}(ik_0+1)$	Computed values of $\hat{y}(ik+1)$ (Richardson extrapolated)
(*a*)		
2^{-4}	0·867 800 33 + i0·000 518 85	
2^{-5}	0·869 680 44 + i0·000 722 21	0·870 307 14 + i0·000 789 99
2^{-6}	0·870 153 12 + i0·000 773 66	0·870 310 68 + i0·000 790 81
2^{-7}	0·870 272 22 + i0·000 786 55	0·870 311 92 + i0·000 790 84
2^{-8}	0·870 302 13 + i0·000 789 79	0·870 312 10 + i0·000 790 86
2^{-9}	0·870 309 64 + i0·000 790 60	0·870 312 15 + i0·000 790 87
2^{-10}	0·870 311 53 + i0·000 790 80	0·870 312 16 + i0·000 790 87
2^{-11}	0·870 312 00 + i0·000 790 85	0·870 312 16 + i0·000 790 87
(*b*)		
2^{-4}	0·802 206 20 + i0·044 450 10	
2^{-5}	0·803 537 82 + i0·045 081 07	0·803 981 69 + i0·045 291 40
2^{-6}	0·803 871 62 + i0·045 240 12	0·803 982 88 + i0·045 293 13
2^{-7}	0·803 955 78 + i0·045 280 05	0·803 983 83 + i0·045 293 36
2^{-8}	0·803 976 91 + i0·045 290 10	0·803 983 95 + i0·045 293 44
2^{-9}	0·803 982 22 + i0·045 292 62	0·803 983 99 + i0·045 293 46
2^{-10}	0·803 983 55 + i0·045 293 25	0·803 983 99 + i0·045 293 46
2^{-11}	0·803 983 88 + i0·045 293 41	0·803 983 99 + i0·045 293 46

Table 2. Convergence of the phase-shift estimates for the static potential $V=-2(1+1/r)\exp(-2r)$. The wavenumber is $k=3$. Equations (3.11) and (3.12) are treated according to the trapezoidal scheme. The backward recursive procedure (§ 3.1.2) is implemented. h is the step size. All results have been Richardson extrapolated once.

h	δ_0	δ_{12}	δ_{18}
2^{-4}	0·571 004 2	0·146 161 1	0·858 762 7
2^{-5}	0·572 661 5	0·000 634 0	0·011 944 8
2^{-6}	0·572 660 6	0·000 230 0	0·000 735 7
2^{-7}	0·572 661 1	0·000 203 6	0·000 050 2
2^{-8}		0·000 201 8	0·000 007 2
2^{-9}		0·000 201 6	0·000 004 63
2^{-10}			0·000 004 47

Table 3. A comparison of three different numerical strategies for the Yukawa potential problem: $\mu_0 = 0$, $\lambda_0 = 1{\cdot}5$, $k_0 = 0{\cdot}5$, $l = 3$. The computed values of the phase shift δ_3 are displayed; h is the step size.

h	$k_0 = 0{\cdot}5$	$l = 3$	
2^{-4}	0·056 717 36	−0·003 981 75	−0·002 020 10
2^{-5}	0·004 411 53	0·002 143 58	0·002 112 32
2^{-6}	0·002 193 56	0·001 982 29	0·002 050 16
2^{-7}	0·002 079 28	0·002 033 57	0·002 030 17
2^{-8}	0·002 033 05	0·002 028 26	0·002 029 00
2^{-9}	0·002 029 65	0·002 028 71	0·002 028 63
2^{-10}	0·002 028 71	0·002 028 59	0·002 028 61
2^{-11}	0·002 028 62	0·002 028 60	0·002 028 60
2^{-12}	0·002 028 61	0·002 028 60	0·002 028 60

Table 4. The S-wave exponential potential problem: $\mu_0 = 1$, $\lambda_0 = 0$, $k_0 = 1$, $l = 0$. h is the step size. Computed values of the phase shift δ_0 are displayed. The exact value is $\delta_0 = 1{\cdot}208\,554\,15\ldots$.

h	2^{-4}	2^{-5}	2^{-6}	2^{-7}
δ_0	1·208 581 04	1·208 554 47	1·208 554 10	1·208 554 16

results may be due to the 'most straightforward' matching routine at $\tilde{r}$, which has been used by Coleman and Mohamed.

Finally, in table 6 for some specific examples a comparison is performed with results obtained by Common (1979, table 1 there) using Klozenberg's (1974) PHASE code for the variable phase equation. Our results refer to the implementation of the trapezoidal scheme on problem (3.1) of I, followed by the forward recursive procedure (§ 3.1.1). In contrast with the behaviour exhibited in table 2, here convergence is quite slow when l is large. The authors are now working on the implementation of faster numerical schemes on a class of functional differential problems which includes problem (3.1) of I and problem (3.11) here.

5. Conclusions

Asymptotic results concerning the Laplace transformation have been employed to derive a convergent numerical scheme for the S-matrix problem for a class of potentials—equation (1.2)—which appear frequently in nuclear physics as well as in atomic physics. Several numerical tests have been performed. Satisfactory convergence properties and good agreements with literature results have been demonstrated.

Appendix

Here we summarise some results concerning an initial-value problem for a linear non-singular neutral functional differential equation on a finite interval for a complex-valued function. Details will be presented elsewhere. Pertinent existence results may

Table 5. Comparisons with the phase-shift calculations of Coleman and Mohamed (1979) for the static potential problem $V=-2(1+1/r)\exp(-r)$. The computation of Coleman and Mohamed involves first the solution of the radial Schrödinger equation on the interval $(0, \tilde{r})$ and then the use of a standard fitting procedure at $\tilde{r}$. (*a*) $l=0$, $k=0{\cdot}5$; (*b*) $l=1$, $k=1{\cdot}0$; (*c*) $l=2$, $k=0{\cdot}4$; (*d*) $l=2$, $k=0{\cdot}5$.

	Our results	Coleman and Mohamed (1979)	
	h	$\tilde{r}$	
(*a*)			
	2^{-4}	$1{\cdot}041\,353$	
	2^{-5}	$1{\cdot}044\,658$	$9{\cdot}242$ $1{\cdot}044\,66$
	2^{-6}	$1{\cdot}044\,658$	$10{\cdot}41$ $1{\cdot}044\,65$
(*b*)			
	2^{-4}	$1{\cdot}112\,935\times10^{-1}$	
	2^{-5}	$1{\cdot}114\,754\times10^{-1}$	$8{\cdot}466$ $1{\cdot}114\,69\times10^{-1}$
	2^{-6}	$1{\cdot}114\,741\times10^{-1}$	$9{\cdot}521$ $1{\cdot}114\,68\times10^{-1}$
	2^{-7}	$1{\cdot}114\,738\times10^{-1}$	
	2^{-8}	$1{\cdot}114\,738\times10^{-1}$	
(*c*)			
	2^{-5}	$5{\cdot}246\,193\times10^{-4}$	
	2^{-6}	$5{\cdot}245\,159\times10^{-4}$	$9{\cdot}915$ $5{\cdot}240\,71\times10^{-4}$
	2^{-7}	$5{\cdot}244\,270\times10^{-4}$	$11{\cdot}23$ $5{\cdot}236\,81\times10^{-4}$
	2^{-8}	$5{\cdot}244\,185\times10^{-4}$	$12{\cdot}54$ $5{\cdot}217\,90\times10^{-4}$
	2^{-9}	$5{\cdot}244\,163\times10^{-4}$	$13{\cdot}82$ $5{\cdot}204\,66\times10^{-4}$
	2^{-10}	$5{\cdot}244\,161\times10^{-4}$	$14{\cdot}84$ $5{\cdot}205\,09\times10^{-4}$
(*d*)			
	2^{-5}	$1{\cdot}390\,750\times10^{-3}$	
	2^{-6}	$1{\cdot}390\,440\times10^{-3}$	$9{\cdot}703$ $1{\cdot}388\,00\times10^{-3}$
	2^{-7}	$1{\cdot}390\,321\times10^{-3}$	$10{\cdot}95$ $1{\cdot}386\,97\times10^{-3}$
	2^{-8}	$1{\cdot}390\,310\times10^{-3}$	$11{\cdot}99$ $1{\cdot}386\,95\times10^{-3}$
	2^{-9}	$1{\cdot}390\,307\times10^{-3}$	
	2^{-10}	$1{\cdot}390\,307\times10^{-3}$	

be found in Furi *et al* (1980). A comprehensive treatment of functional equations with delays may be found in Hale (1977). Some numerical methods have been reviewed by Cryer (1972).

The problem is†

$$y^{(1)}(x)=a(x)y^{(1)}(\alpha(x))+b(x)y(x)+c(x)y(\alpha(x))+u(x), \qquad x\in[0,1], \tag{A1a}$$

$$y(0)=y^0\in\mathbb{C}, \tag{A1b}$$

$$y\in\mathscr{C}^m([0,1],\mathbb{C}), \tag{A1c}$$

where $y^{(k)}(x)=\mathrm{d}^k y(x)/\mathrm{d}x^k$ $(k=1,2,\ldots)$ and where m is some positive integer. It is assumed that the parameters α, a, b, c and u obey the requirements

$$\alpha, a, b, c, u\in\mathscr{C}^{m-1}([0,1],\mathbb{C}), \tag{A2a}$$

† When $a(x)\equiv 0$ for $x\in[0,1]$, problem (A1) reduces to the retarded (or delayed) problem discussed, for instance, by Feldstein (1964, see also appendix 2 of Paiano and Paveri-Fontana 1978).

Table 6. Comparison with the phase-shift calculation performed by Common (1979) for the Yukawa potential $V=-(4/r)\exp(-r)$, with $k^2=45$. Common solves numerically the variable phase equation, using a code due to Klozenberg (1974).

h	δ_0	δ_3	δ_5	δ_7	δ_{12}
2^{-4}	0·774 27	0·259 10	0·351 26		
2^{-5}	0·791 82	0·274 86	0·230 55		
2^{-6}	0·791 21	0·270 66	0·214 04	0·698 60	
2^{-7}	0·791 16	0·269 62	0·210 43	0·221 56	
2^{-8}	0·791 16	0·269 38	0·209 51	0·134 50	
2^{-9}		0·269 31	0·209 29	0·113 84	0·995 52
2^{-10}		0·269 30	0·209 23	0·108 92	0·730 91
2^{-11}			0·209 22	0·107 68	0·343 35
2^{-12}				0·107 38	0·129 64
2^{-13}				0·107 30	0·063 60
2^{-14}				0·107 28	0·046 23
2^{-15}					0·041 84
2^{-16}					0·040 74
Common (1979)	0·791 2	0·269 3	0·209 2	0·107 3	0·040 4

$$0<\alpha(x)<x, \qquad x\in(0,1], \tag{A2b}$$

$$|a(0)|<1, \tag{A2c}$$

$$|a(0)\alpha^{(k)}(0)|<1, \qquad k\in\{0,1,\ldots,m-1\}. \tag{A2d}$$

For $m\geq 3$, under the additional assumption

$$\mathrm{d}\alpha(x)/\mathrm{d}x>0, \qquad x\in[0,1], \tag{A3}$$

a numerical scheme for the problem is suggested by integrating by parts equation (A1a) on the interval $(x, x+h)$:

$$y(x+h)-y(x)=\beta(x+h)y(\alpha(x+h))-\beta(x)y(\alpha(x)) + \int_x^{x+h}\left(b(\xi)y(\xi)+\left(c(\xi)-\frac{\mathrm{d}}{\mathrm{d}\xi}\beta(\xi)\right)y(\alpha(\xi))\right)\mathrm{d}\xi, \tag{A4}$$

where

$$\beta(x)=\frac{a(x)}{\mathrm{d}\alpha(x)/\mathrm{d}x}, \qquad x\in[0,1].$$

We partition the interval $[0,1]$ in N intervals of length $h=1/N$ and we set $x_k=kh$, $\alpha_k=\alpha(x_k)$, $\beta_k=\beta(x_k)$, $\beta'_k=\beta^{(1)}(x_k)$, $a_k=a(x_k)$, $b_k=b(x_k)$, $c_k=c(x_k)$, and

$$q_{(k)}=[\alpha(x_k)/h], \qquad r_k=\alpha(x_k)/h-q_{(k)},$$

where $[u]$ denotes the largest integer that is smaller than (or equal to) u. In addition, by linear interpolation, we take

$$z_k=(1-r_k)y_{q(k)}+r_k y_{q(k)+1}$$

as an approximation for $y(\alpha(x_k))$. Here, of course, y_k is the counterpart of $y(x_k)$.

Applying the trapezoidal scheme to the RHS of (A4) we obtain a 'trapezoidal' fixed-step algorithm for problem (A1):

$$y_0 = y^0,$$

$$y_{k+1} = y_k + (\beta_{k+1} z_{k+1} - \beta_k z_k) + \tfrac{1}{2}h((b_{k+1} y_{k+1} + b_k y_k) + (c_{k+1} - \beta'_{k+1}) y_{k+1} + (c_k - \beta'_k) y_k), \qquad k \in \{0, 1, \ldots, N-1\}. \tag{A5}$$

We shall make use of the following notation. For $k \in \{1, 2, \ldots, N\}$, $x \in [0, 1]$ and $h = 1/N$, $y(x)$ and $y_{k,h}$ denote the solutions of (A1) and (A5), respectively; moreover

$$\tilde{y}_{k,h} = \tfrac{1}{7}(8 y_{2k,h/2} - y_{k,h}) \tag{A6}$$

is the Richardson extrapolated version of $y_{k,h}$. Finally, by linear interpolation, for all $x \in [0, 1]$ we set

$$y(x, h) = (x/h - [x/h]) y_{[x/h]+1,h} + ([x/h] + 1 - x/h) y_{[x/h]}, \tag{A7}$$

$$\tilde{y}(x, h) = (x/h - [x/h]) \tilde{y}_{[x/h]+1,h} + ([x/h] + 1 - x/h) \tilde{y}_{[x/h]}. \tag{A8}$$

We have:

Proposition 1. Let (A2) hold for some integer $m \geqslant 1$. Then problem (A1) admits one and only one solution.

Proposition 2. Let (A2) and (A3) hold for some integer $m \geqslant 3$. Then there are constants K_1 and N_1 such that for any integer $N \geqslant N_1$ problem (A5), with $h = 1/N$, admits a unique solution, and

$$|y(x) - y(x, h)| \leqslant K_1 h^2, \qquad x \in [0, 1].$$

In addition, if $m \geqslant 4$, there are positive constants K_2 and N_2 such that for any integer $N \geqslant N_2$, with $h = 1/N$, one has

$$|\tilde{y}(x) - \tilde{y}(x, h)| < K_2 h^3, \qquad x \in [0, 1].$$

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