

## Improved continued fraction treatment of the one-dimensional scattering problem

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1981 J. Phys. A: Math. Gen. 14 1815

(<http://iopscience.iop.org/0305-4470/14/7/035>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 129.252.86.83

The article was downloaded on 30/05/2010 at 14:40

Please note that [terms and conditions apply](#).

COMMENT

## Improved continued fraction treatment of the one-dimensional scattering problem

Ph Lambin and J P Vigneron

Institut de Physique, B5, Université de Liège, B-4000 Sart Tilman/Liège 1, Belgium

Received 9 October 1980, in final form 25 November 1980

**Abstract.** The Numerov discretisation scheme is used to obtain a numerical solution of the one-dimensional scattering problem for an arbitrary potential barrier. The three-term recursion obtained from this scheme is treated by using a continued fraction technique in order to extract an explicit expression of the transmission coefficient and the phaseshift. The efficiency of the method is discussed.

In a recent paper (Vigneron and Lambin 1980, hereafter referred to as VL) a numerical method for computing the transmission coefficient in one-dimensional scattering problems has been presented. The aim of this comment is a new formulation of the problem in order to obtain not only the transmission coefficient but also the wavefunction phaseshift. Furthermore the precision has been considerably improved by discretisation of the Schrödinger equation

$$\frac{d^2\psi(x)}{dx^2} = (v(x) - \varepsilon)\psi(x) \quad (1)$$

using the Numerov method (Numerov 1924) rather than the simple second-order difference equation considered in VL. The Numerov method gives rise to the following finite difference equation

$$\begin{aligned} [1 - \frac{1}{12}h^2(v(x_{p+1}) - \varepsilon)]\psi(x_{p+1}) - [2 + \frac{5}{6}h^2(v(x_p) - \varepsilon)]\psi(x_p) \\ + [1 - \frac{1}{12}h^2(v(x_{p-1}) - \varepsilon)]\psi(x_{p-1}) = 0 \end{aligned} \quad (2)$$

when the  $x_p$  form a grid of equidistant points separated by the step  $h$ . The truncation error in equation (2) is proportional to  $h^4$ . The Numerov method has been rather widely used to solve for the bound states of the radial Schrödinger equation encountered in molecular or nuclear physics (see, for instance, Hajj 1974). For our purpose we take advantage of the fact that equation (2) is still a three-term recursion so that the continued fraction technique can be used along the same lines described in VL.

It will be assumed that the potential energy  $v(x)$  is constant and equal to zero outside the interval  $]x_0, x_{n+1}[$ . Following VL we look for a solution of the finite difference equation (2) which satisfies the conditions

$$\psi(x_p) = A[R^-]^{|p|} + B[R^+]^{|p|} \quad (3)$$

for  $p \leq 0$  and

$$\psi(x_p) = [R^+]^{p-n-1} \quad (4)$$

for  $p \geq n + 1$ . In these expressions,  $R^+$  and  $R^-$  are given by

$$R^\pm = \frac{1 - \frac{5}{12}h^2\varepsilon}{1 + \frac{1}{12}h^2\varepsilon} \pm i \left[ 1 - \left( \frac{1 - \frac{5}{12}h^2\varepsilon}{1 + \frac{1}{12}h^2\varepsilon} \right)^2 \right]^{1/2} \quad (5)$$

which are complex conjugate in the energy range  $0 < \varepsilon < 6/h^2$ . The problem is solved once the coefficients  $A$  and  $B$  involved in equation (3) are known. A first relation between  $A$  and  $B$  is easily obtained in the form (see VL for details)

$$\frac{AR^- + BR^+}{A + B} = \frac{R^-A_{n+2} - a_{n+1}(\varepsilon)A_{n+1}}{R^-B_{n+1} - a_{n+1}(\varepsilon)B_n} \quad (6)$$

where the  $A_{p+1}$  and  $B_p$  are constructed recursively by

$$A_{p+1} = b_p(\varepsilon)A_p - a_{p-1}(\varepsilon)A_{p-1} \quad (7)$$

$$B_p = b_p(\varepsilon)B_{p-1} - a_{p-1}(\varepsilon)B_{p-2} \quad (8)$$

for  $p = 2, 3, \dots, n + 1$ , with the starting values

$$A_1 = b_0(\varepsilon) \quad A_2 = b_1(\varepsilon)b_0(\varepsilon) - a_0(\varepsilon) \quad (9)$$

$$B_0 = 1 \quad B_1 = b_1(\varepsilon). \quad (10)$$

The  $a_p(\varepsilon)$  and  $b_p(\varepsilon)$  which appear in the last equations are the partial numerators and denominators of the continued fraction generated from the recurrence

$$R_{p-1} = b_p(\varepsilon) - a_p(\varepsilon)/R_p \quad (11)$$

between the ratios  $R_p$  of the wavefunction values at two successive grid points  $x_p$  and  $x_{p+1}$  and are easily deduced from equation (2). A second independent relation between  $A$  and  $B$  can be found by noticing that

$$\psi(x_0) = \psi(x_{n+1}) \prod_{p=0}^n R_p. \quad (12)$$

Using a theorem which has been demonstrated in the appendix of a previous paper (Vigneron and Lambin 1979) and after some simple mathematical transformations equation (12) yields

$$A + B = \frac{R^-B_{n+1} - a_{n+1}(\varepsilon)B_n}{R^-}. \quad (13)$$

The transmission coefficient  $T$  and the phaseshift  $\varphi$  are defined respectively as the square modulus and the phase of the complex quantity  $1/A$ . Combining equations (6) and (13) gives the following explicit formula

$$\sqrt{T}e^{i\varphi} \equiv \frac{1}{A} = \frac{R^+ - R^-}{a_{n+1}(\varepsilon)R^+C_{n+1} - C_{n+2}} \quad (14)$$

where the complex quantities

$$C_{p+1} = A_{p+1} - R^+B_p \quad (15)$$

can be recursively constructed using a recursion identical to that defined by equations (7) or (8).

The use of the Numerov method implicitly supposes that the potential energy  $v(x)$  is doubly differentiable. In the case where a jump of potential occurs at a grid point  $x_p$ , the

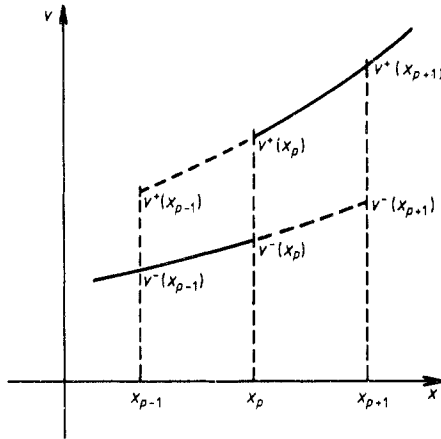
method may still be used by an adaptation of the coefficients  $a_p(\epsilon)$  and  $b_p(\epsilon)$  which connect  $R_{p-1}$  and  $R_p$ . By Taylor expansions of  $\psi(x_p - h)$  and  $\psi(x_p + h)$  and by imposing the continuity of the logarithmic derivative of the wavefunction at  $x_p$ , one again finds relation (11) with

$$a_p(\epsilon) = \frac{1 - \frac{1}{12}h^2(\frac{3}{2}v^+(x_{p+1}) - \frac{1}{2}v^-(x_{p+1}) - \epsilon)}{1 - \frac{1}{12}h^2(\frac{3}{2}v^-(x_{p-1}) - \frac{1}{2}v^+(x_{p-1}) - \epsilon)} \tag{16}$$

and

$$b_p(\epsilon) = \frac{2 + \frac{5}{6}h^2(\frac{1}{2}v^+(x_p) + \frac{1}{2}v^-(x_p) - \epsilon)}{1 - \frac{1}{12}h^2(\frac{3}{2}v^-(x_{p-1}) - \frac{1}{2}v^+(x_{p-1}) - \epsilon)}. \tag{17}$$

It has been assumed that the potential energy is equal to  $v^-(x)$  left of the  $x_p$  and equal to  $v^+(x)$  right of  $x_p$  as shown in figure 1. In the case where no discontinuity occurs, equations (16) and (17) reduce to the expressions of  $a_p(\epsilon)$  and  $b_p(\epsilon)$  deduced from the recursion (2).



**Figure 1.** A discontinuity of the potential at a grid point  $x_p$  requires an adaptation of the Numerov discretisation scheme.

As an application of the method we consider again the square top barrier already solved in VL

$$v(x) = 10 \tag{18}$$

for  $0 < x < 2$  and

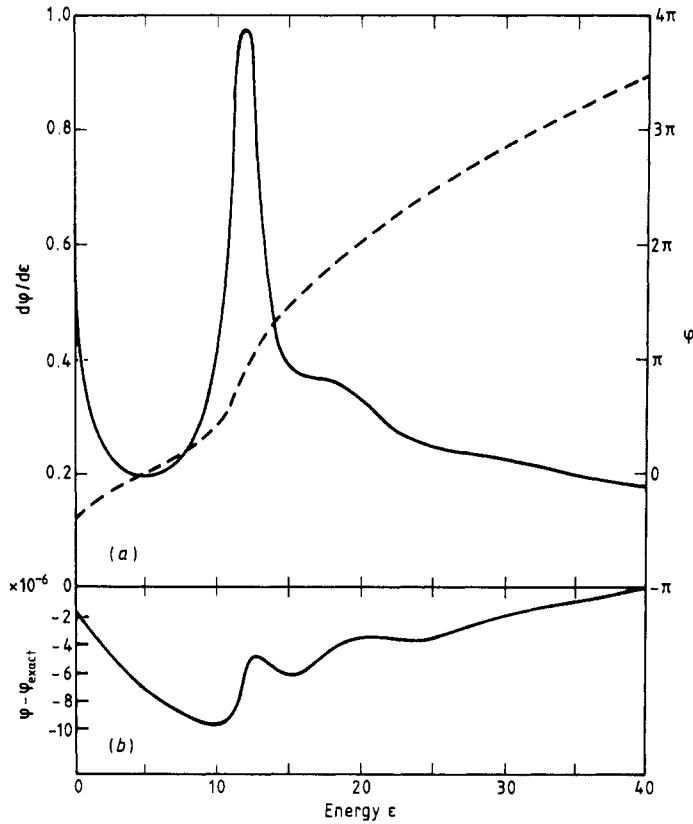
$$v(x) = 0 \tag{19}$$

for  $x < 0$  and  $x > 2$ . Table 1 shows how the convergence of the transmission coefficient and the phaseshift toward the exact values (Schiff 1955) is fairly fast. As compared with VL, a substantial increase in precision is found. Figure 2 represents the phaseshift and its derivative with respect to the energy in the case where  $n = 100$ . The derivative of the phaseshift with respect to energy is interesting because closely related to the quantum

tunnelling time (Messiah 1969). This is especially important for the investigation of resonant states in the continuous spectrum of the one-dimensional Hamiltonian. An interesting description of this can be found in Goldberg *et al* (1967).

**Table 1.** Convergence of the transmission coefficient and of the phaseshift for different discretisation step sizes of the square-top potential barrier.

Energy $\epsilon$		0.5	5	20
Transmission coefficient	$n = 10$	$0.330\ 672 \times 10^{-5}$	$0.515\ 719 \times 10^{-3}$	0.999 688
	$n = 50$	$0.336\ 052 \times 10^{-5}$	$0.521\ 734 \times 10^{-3}$	0.999 785
	$n = 100$	$0.336\ 098 \times 10^{-5}$	$0.521\ 786 \times 10^{-3}$	0.999 786
	$n = 200$	$0.336\ 103 \times 10^{-5}$	$0.521\ 793 \times 10^{-3}$	0.999 786
	Exact	$0.336\ 104 \times 10^{-5}$	$0.521\ 794 \times 10^{-3}$	0.999 786
Phaseshift	$n = 10$	-1.121 11	$-0.558\ 281 \times 10^{-2}$	6.325 85
	$n = 50$	-1.119 78	$-0.561\ 872 \times 10^{-4}$	6.327 04
	$n = 100$	-1.119 77	$-0.723\ 432 \times 10^{-5}$	6.327 06
	$n = 200$	-1.119 77	$-0.917\ 858 \times 10^{-6}$	6.327 06
	Exact	-1.119 77	0.0	6.327 06



**Figure 2.** (a) Phaseshift (broken curve) and its derivative with respect to the energy (full curve) for the square-top potential barrier. (b) Absolute deviation of the phaseshift from the exact result:  $\phi - \phi_{\text{exact}}$ .

### **Acknowledgments**

Both authors acknowledge the Belgian Fonds National de la Recherche Scientifique for financial support.

### **References**

- Goldberg A, Schey H M and Schwartz J L 1967 *Am. J. Phys.* **35** 177  
Hajj F Y, Kobeisse H and Nassif N R 1974 *J. Comput. Phys.* **16** 150  
Messiah A 1969 *Mécanique Quantique* (Paris: Dunod)  
Numerov B V 1924 *Mon. Not. R. Astron. Soc.* **84** 592  
Schiff L I 1955 *Quantum Mechanics* (New York: McGraw-Hill)  
Vigneron J P and Lambin Ph 1979 *J. Phys. A: Math. Gen.* **12** 1961  
— 1980 *J. Phys. A: Math. Gen.* **13** 1135