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An asymmetric form of the discrete Schrödinger equation with application to the inverse tunnelling problem†

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Abstract. If the solution of the Schrödinger equation at one boundary joins smoothly to a plane wave, then from the knowledge of the logarithmic derivative of the wavefunction at the other boundary one can determine the potential between these two boundaries. In this paper a discrete method of solving the inverse problem for potentials of finite range is discussed where the frequency-dependent logarithmic derivative of the wavefunction is fitted at N points using Thiele's reciprocal difference method. This fit is compatible with the solution obtained from an asymmetric discrete form of the wave equation. By comparing the logarithmic derivatives found from the fit and calculated from the difference equation, one can determine the potential. The method has been tested on two exactly solvable problems.

1. Introduction

Symmetric forms of difference equations approximating a given differential equation have been studied by a number of authors in connection with the inverse problems of quantum scattering theory and of the wave propagation (Case and Kac 1973, Zakhar'ev *et al* 1977, Hron and Razavy 1977, 1979, Berryman and Greene 1978). In these formulations one deals with a real input function, namely, the phaseshift, or a related quantity, the logarithmic derivative of the wavefunction outside the range of the potential. This latter quantity is also real and can be expressed as the ratio of two polynomials. According to the way that one formulates the problem, the variable in these polynomials is either $k^2\Delta^2$ or $\cos k\Delta$, where k and Δ are the wavenumber and the element of length (the difference operator) respectively. A source of difficulty in the application of these methods is that of fitting the input data in such a way that the resulting expression for the logarithmic derivative turns out to be compatible with the corresponding form found from the solution of the difference equation. In the cases where the phaseshift is known analytically, or the logarithmic derivative of the wavefunction is obtained from the solution of the direct problem, this difficulty is not serious. But if the data are known as a series of measured points, then a general Padé approximant $[L/M]$ (Baker 1975) can be used to find a fit to the logarithmic derivative of the wavefunction only if the generating difference equation for the approximants can be related to the Schrödinger equation. In this work we choose a special form of the Padé approximant, namely, Thiele's reciprocal difference method (Milne-Thomson

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1951, Baker 1975) to fit the input data. Other Padé-type fits may be more appropriate when certain aspects of the available information need to be emphasised, e.g., the correct asymptotic behaviour as a function of k, or the least-squares fit of approximating the input data (Miller 1970). Here Thiele's method is chosen on account of its simplicity and its compatibility with the solution of a simple difference equation. Since the Padé approximant resulting from this fit cannot be used in conjunction with the previously considered symmetric forms of the difference equation, we have studied the possibility of reformulating the discrete version of the wave equation by replacing the symmetric forms by an asymmetric one. By an asymmetric difference equation we mean an equation whose generating (tri-diagonal) matrix is not symmetric. This asymmetric difference equation reduces to the Schrödinger equation in the limit of $\Delta \to 0$, and $N \to \infty$, and can be used with the Padé approximant obtained by Thiele's rational fraction fit. In this case the polynomials are functions of the complex variable $\zeta^2 - 2\zeta$ where $\zeta = \exp(-ik\Delta)$. Since the wave amplitude now is a function of the complex variable $\zeta^2 - 2\zeta$, the method is applicable to the cases where the solution of the Schrödinger equation is complex. For instance, the inverse problem of reflection and transmission through a potential barrier or inverse scattering by complex potentials are among those that can be solved by this method.

The Schrödinger equation and its corresponding asymmetric difference equation and their boundary conditions are studied in § 2 of the present paper. In § 3 two solvable models of the Schrödinger equation are discussed, and from their exact solutions, the ratio of the wavefunction at two neighbouring points and also their logarithmic derivatives at one of the boundaries are obtained. These are used to test the validity and the accuracy of replacing the Schrödinger equation by a finite-difference equation. In § 4 the pointwise fit of the input data is discussed when the logarithmic derivative of the wavefunction is given for a number of frequencies. For the two solvable models, the results of the direct and the inverse problems are found and compared with the exact result in § 5.

2. A discrete form of the wave equation

Let us consider a one-dimensional problem where a potential barrier partially reflects and partially transmits the incident wave. We assume that the potential barrier, which extends from $x = c$ to a finite range b, is continuous everywhere except at $x = c$. In the direct problem, from the potential $v(x)$ one determines the coefficients of reflection and transmission for this barrier. In the inverse problem the logarithmic derivative of the wavefunction at $x = c$ is given as a function of the wavenumber and the object is to construct the potential from this logarithmic derivative. To solve the direct problem we start with the Schrödinger equation

$$\psi'' + (k^2 - v(x))\psi = 0 \tag{2.1}$$

where primes denote derivatives with respect to x. The solution of (2.1) in the two regions $x < c$ and $x > c$ can be written as

$$\psi = A\,\mathrm{e}^{ikx} + B\,\mathrm{e}^{-ikx} \qquad x < c \tag{2.2}$$

and

$$\psi = Cf(k, x) \qquad x > c \tag{2.3}$$

where $f(k, x)$ is the solution of (2.1) with the boundary condition

$$\lim_{x\to\infty} f(x) \to e^{ikx}. \tag{2.4}$$

At $x = c$ the logarithmic derivatives of (2.2) and (2.3) should be equal, i.e.

$$Z(k) = ik(A - B\, e^{-2ikc})/(A + B\, e^{-2ikc}) = f'(k, c)/f(k, c). \tag{2.5}$$

Solving (2.5) for B/A we find the reflection amplitude:

$$B/A = e^{2ikc}\left(1 + \frac{i}{k}\frac{f'(k, c)}{f(k, c)}\right)\left(1 - \frac{i}{k}\frac{f'(k, c)}{f(k, c)}\right)^{-1}. \tag{2.6}$$

Now let us formulate the discrete version of this problem. Generally the difference equation which replaces the Schrödinger equation is written in a symmetric way, i.e. f'' is approximated by $\Delta^{-2}(f_{n+1} + f_{n-1} - 2f_n)$ where Δ is the difference interval. But this replacement is not unique; other symmetric or asymmetric difference equations can be found that reduce to the Schrödinger equation as $\Delta \to 0$, and have the same percentage of error. The particular form that will be considered in this paper is

$$f_{n-1}(\zeta) = 2f_n(\zeta) + (\zeta^2 - 2\zeta)\exp(-\Delta^2 v_n) f_{n+1}(\zeta) \tag{2.7}$$

where

$$\zeta = \exp(-ik\Delta). \tag{2.8}$$

As far as we know this form has not been used before, and the best argument for its use is the close agreement between the results obtained with this form and from the exact solution of the Schrödinger equation.

We observe that in the limit of $\Delta \to 0$, this difference equation can be written as

$$\Delta^{-2}(f_{n+1} + f_{n-1} - 2f_n) = -(k^2 - v_n) f_{n+1} \tag{2.9}$$

and hence as $\Delta \to 0$, (2.7) goes over to the differential equation (2.1) or

$$f'' + (k^2 - v(x))f = 0. \tag{2.10}$$

For large values of x, $v(x)$ tends to zero; therefore in the discrete version we have

$$v_n = 0 \qquad \text{for } n \geq N \tag{2.11}$$

where $N\Delta = b - c$ represents the range of the potential, i.e. for $x \geq N\Delta + c$ the potential is either zero or negligibly small. Thus for $n \geq N$ (2.7) reduces to

$$f_{n-1} = 2f_n + (\zeta^2 - 2\zeta) f_{n+1} \tag{2.12}$$

which has two independent solutions

$$f_n = \zeta^{-n} = \exp(ik\Delta n) \qquad n > N \tag{2.13}$$

or

$$f_n = (2 - \zeta)^{-n} \qquad n > N. \tag{2.14}$$

The boundary condition (2.4) shows that (2.13) is the acceptable solution of (2.12). Now let us change f_n to F_n where

$$F_n = 2^n f_n; \tag{2.15}$$

then the difference equation (2.7) changes to

$$F_{n-1} = F_n + \tfrac{1}{4}(\zeta^2 - 2\zeta)\exp(-\Delta^2 v_n) F_{n+1}. \tag{2.16}$$

This difference equation used with the boundary condition

$$F_n = 2^n\, e^{ikn\Delta} = 2^n \zeta^{-n} \qquad n \geqslant N \tag{2.17}$$

enables us to write f_0/f_1 as a continued J fraction (Wall 1948)

$$\frac{f_0}{2f_1} = \frac{F_0}{F_1} = 1 + \frac{\frac{1}{4}(\zeta^2 - 2\zeta)\, e^{-\Delta^2 v_1}}{1+}\,\frac{\frac{1}{4}(\zeta^2 - 2\zeta)\, e^{-\Delta^2 v_2}}{1+}\,\frac{\frac{1}{4}(\zeta^2 - 2\zeta)\, e^{-\Delta^2 v_3}}{1+}\dots \tag{2.18}$$

Thus the quantity that corresponds to the logarithmic derivative in this formulation is given by the relation

$$Z_N(\zeta) = \Delta^{-1}(1 - f_0/f_1). \tag{2.19}$$

For solving the direct problem we start with equation (2.16) for $n = N$ and $n = N+1$, and note that since $v_n = 0$, according to equation (2.17), we have

$$\frac{F_N}{F_{N+1}} = \tfrac{1}{2}\zeta = \tfrac{1}{2}\{1 - [1 + (\zeta^2 - 2\zeta)]^{1/2}\} \tag{2.20}$$

and

$$\frac{F_{N-1}}{F_N} = 1 + \tfrac{1}{4}(\zeta^2 - 2\zeta)\exp(-\Delta^2 v_N)\frac{F_{N+1}}{F_N}. \tag{2.21}$$

Equations (2.20) and (2.21) enable us to calculate F_{n-1}/F_n for any value of n from the recursion relation

$$\frac{F_{n-1}}{F_n} = 1 + \tfrac{1}{4}(\zeta^2 - 2\zeta)\exp(-\Delta^2 v_n)\frac{1}{(F_n/F_{n+1})}. \tag{2.22}$$

In this way we can calculate F_0/F_1 by N iterations and then determine $Z_N(\zeta)$ from (2.19). Because of the boundary condition (2.20) F_0/F_1 is a function of ζ and not $\zeta^2 - 2\zeta$ which is the parameter appearing in the difference equation (2.22). However, for any rational approximation of (2.20) in terms of $\zeta^2 - 2\zeta$, F_0/F_1 and consequently $Z_N(\zeta)$ will depend on $\zeta^2 - 2\zeta$.

3. Examples

We can test the accuracy of the approximate form of $Z(\zeta)$ calculated from (2.19) by comparing $Z_N(\zeta)$ obtained by numerical calculation with the corresponding quantity $Z(k)$ (equation (25)) derived from the exact solution of the Schrödinger equation. For this purpose we consider two solvable models where in each model $Z(k)$ is given in terms of elementary functions. In the first model the potential decreases exponentially for large x and the Schrödinger equation is given by

$$\psi'' + k^2\psi = 2\nu\mu^2\, e^{-\mu x}\psi/(1 - \nu\, e^{-\mu x})^2 \qquad \nu < 1. \tag{3.1}$$

For this case we choose b to be a number much larger than $1/\mu$ and take $c = 0$. The solution of (3.1) subject to the boundary condition

$$\lim_{x\to\infty} \psi(x)\, e^{-ikx} \to 1 \tag{3.2}$$

is

$$\psi(x) = e^{ikx}[1 + 2\nu\, e^{-\mu x}/(1 - 2ik/\mu)(1 - \nu\, e^{-\mu x})]. \tag{3.3}$$

From the analytical form of $\psi(x)$, we can calculate $Z(k)=\psi'(0)/\psi(0)$. This quantity is related to the solution of the difference equation $(f_1-f_0)/\Delta f_0$ in the limit of $\Delta\to 0$. Alternatively we can express f_0/f_1 in terms of ψ and its derivative at the origin:

$$f_0/f_1=\psi(0)/(\psi(0)+\Delta\psi'(0)) \tag{3.4}$$

provided that Δ is very small. A better approximation for f_0/f_1 results by noting that

$$f_0=\psi(0) \qquad \text{and} \qquad f_1=\psi(x=\Delta). \tag{3.5}$$

Using these relations and equation (3.3) we find

$$f_0/f_1=\zeta\{(1-\nu)[1+(2/\mu\Delta)\ln\zeta]+2\nu\}/[\![(1-\nu)\{[1+(2/\mu\Delta)\ln\zeta] + 2\nu\,\mathrm{e}^{-\mu\Delta}/(1-\nu\,\mathrm{e}^{-\mu\Delta})\}]\!] \tag{3.6}$$

where ζ is given by (2.8). As a second example we consider the Schrödinger equation

$$\psi''+\left(k^2+\frac{2}{b^2}-\frac{2}{x^2}\right)\psi=0 \qquad c\leqslant x\leqslant b \tag{3.7}$$

with the boundary condition

$$\psi(x)=\mathrm{e}^{\mathrm{i}kx} \qquad x\geqslant b. \tag{3.8}$$

The solution of (3.7) subject to the boundary condition (3.8) is

$$\psi(x)=C\left(\alpha(x)-\frac{\mathrm{i}k\alpha(b)-q\gamma(b)}{\mathrm{i}k\beta(b)+q\delta(b)}\beta(x)\right)=C(\alpha(x)-F\beta(x)) \tag{3.9}$$

where

$$q^2=k^2+2/b^2 \tag{3.10}$$

$$\alpha(x)=\sin qx/(qx)-\cos qx \tag{3.11}$$

$$\beta(x)=\sin qx+\cos qx/(qx) \tag{3.12}$$

$$\gamma(x)=\frac{\cos qx}{qx}-\frac{\sin qx}{(qx)^2}+\sin qx \tag{3.13}$$

and

$$\delta(x)=\frac{\sin qx}{qx}+\frac{\cos qx}{(qx)^2}-\cos qx. \tag{3.14}$$

From equation (3.9) we can calculate the logarithmic derivative of ψ at $x=c$

$$\frac{c\psi_1'(x)}{\psi_1(x)}=\frac{\gamma(c)+F\delta(c)}{\alpha(c)-F\beta(c)} \tag{3.15}$$

where F is defined by (3.9).

4. Pointwise fit of the logarithmic derivative of the wavefunction

Let us assume that the logarithmic derivative of the wavefunction as a function of $\xi=(\zeta^2-2\zeta)^{-1}$ is given for $N+1$ values of ξ, say, $\xi_1,\ldots,\xi_N,\xi_{N+1}$. We can express this logarithmic derivative as a continued fraction by means of Thiele's reciprocal difference method (Milne–Thomson 1951). Let us write

$$Z_N(\xi)=\frac{Z_N(\xi_1)}{1+}\frac{(\xi-\xi_1)a_1}{1+}\frac{(\xi-\xi_2)a_2}{1+}\cdots\frac{(\xi-\xi_N)a_N}{1}. \tag{4.1}$$

From this relation we get a set of $(N-1)$ equations:

$$Z_N(\xi_{j+1})=\frac{Z_N(\xi_1)}{1+}\frac{(\xi_{j+1}-\xi_1)a_1}{1+}\cdots\frac{(\xi_{j+1}-\xi_j)a_j}{1} \qquad j=1,2,\ldots,N. \tag{4.2}$$

Since $Z_N(\xi_{j+1})$, $j=1,\ldots,N$ are given, we solve (4.2) for the coefficients a_j:

$$a_j=(\xi_j-\xi_{j+1})^{-1}\left(1+\frac{(\xi_{j+1}-\xi_{j-1})a_{j-1}}{1+}\frac{(\xi_{j+1}-\xi_{j-2})a_{j-2}}{1+}\cdots\frac{(\xi_{j+1}-\xi_1)a_1}{1-Z(\xi_1)/Z(\xi_{j+1})}\right) \tag{4.3}$$

and

$$a_1=\left(\frac{Z_N(\xi_1)}{Z_N(\xi_2)}-1\right)(\xi_2-\xi_1)^{-1}. \tag{4.4}$$

If we increase the order of approximation from N to $N+1$, all the a remain the same, but a_{N+1} will be added to $Z(\xi)$ in (4.1). The continued fraction (4.1) is generated by the following difference equation

$$s_{n+1}=s_n+(\xi-\xi_n)a_n s_{n-1} \tag{4.5}$$

which has exactly the form of the difference equation (2.16) for F_n. Because of this important property the functional form of $Z_N(\xi)$ will be the same as $Z_N(\zeta^2-2\zeta)$ given by equations (2.18) and (2.19). For even N, $Z_N(\xi)$ is the ratio of two polynomials each of order $\frac{1}{2}N$, whereas for odd N, $Z_N(\xi)$ is the ratio of a polynomial of order $\frac{1}{2}(N-1)$ divided by a polynomial of order $\frac{1}{2}(N+1)$ (Schlessinger 1968, Baker 1975).

5. Results

Starting with the boundary condition (2.20), we can solve the direct problem by iterating (2.22) N times to find F_0/F_1. Then using (2.15) and (2.19) we can calculate $Z_N(\zeta)$. In tables 1 and 2 values of f_0/f_1 are given for the Eckart potential (equation (3.1)) with the parameters $\mu=1$ and $\nu=\frac{1}{3}$. The results of numerical calculation are compared with the analytic solution (3.6) in table 1. The real part of f_0/f_1 is very close to one for all wavenumbers (see equation (3.4)), but the imaginary part varies significantly as k changes. The agreement between the solution of the difference equation (2.22) and the differential equation (3.1) is excellent for all values of k.

To solve the inverse problem we proceed in two different ways. In the first case we calculate f_0/f_1 from the difference equation by iteration as a function of $\zeta^2-2\zeta$. Having obtained a Padé approximant of the form $[\frac{1}{2}(N-1)/\frac{1}{2}(N+1)]$ or $[\frac{1}{2}N/\frac{1}{2}N]$ for this quantity, we invert it using a J-fraction expansion (Wall 1948), and from the coefficients of expansion we determine the potential. This has been done for the Eckart potential in table 2, where the potential input is given at 48 points and after inversion the output potential is obtained at the same 48 points. By comparing the given numbers in this table it is clear that the method works very well for the first 10 points and after that it becomes unreliable because of the accumulation of errors. It is remarkable that the unreliable results are for the points where the potential is already very small. For the

Table 1. The real and imaginary parts of f_0/f_1 calculated for the Eckart potential using equations (3.6) and (2.18) respectively. The parameters used in this calculation are $N=5000$, $\Delta=4\times10^{-3}$, $\mu=1$ and $\nu=\frac{1}{3}$.

	Exact		$f_N/f_{N+1}=\zeta$	
κ	$\mathrm{Re}(f_0/f_1)$	$\mathrm{Im}(f_0/f_1)$	$\mathrm{Re}(f_0/f_1)$	$\mathrm{Im}(f_0/f_1)$
0.100 000E-02	1.000 29	−0.157 213E-06	1.000 30	−0.399 820E-06
0.100 000E-01	1.000 29	−0.157 221E-05	1.000 30	−0.397 119E-05
0.500 000E-01	1.000 29	−0.787 077E-05	1.000 30	−0.192 559E-04
0.100 000	1.000 29	−0.158 025E-04	1.000 30	−0.370 117E-04
0.500 000	1.000 25	−0.889 353E-04	1.000 28	−0.129 457E-03
0.750 000	1.000 20	−0.153 079E-03	1.000 23	−0.171 871E-03
1.000 00	1.000 15	−0.239 382E-03	1.000 15	−0.250 075E-03
2.500 00	1.000 04	−0.889 589E-03	1.000 01	−0.953 223E-03
5.000 00	1.000 01	−0.194 483E-02	0.999 999	−0.198 802E-02
7.500 00	0.999 998	−0.296 059E-02	0.999 996	−0.299 467E-02
10.000 0	0.999 997	−0.396 911E-02	0.999 992	−0.399 699E-02
25.000 0	0.999 950	−0.998 894E-02	0.999 950	−0.999 935E-02
50.000 0	0.999 797	−0.199 939E-01	0.999 800	−0.199 985E-01
75.000 0	0.999 527	−0.299 877E-01	0.999 550	−0.299 954E-01
100.000	0.998 827	−0.395 426E-01	0.999 200	−0.399 893E-01

Table 2. Numerical determination of the Eckart potential from f_0/f_1. This latter quantity as a function of $\zeta^2-2\zeta$ is calculated from (2.18). The input data $V(N)$ and the output *VINV* are compared for a number of points. The parameters used in this calculation are $N=48$, $\Delta=0.35$, $\mu=1$ and $\nu=\frac{1}{3}$.

		$f_N/f_{N+1}=\zeta$	
$X(N)$	$V(N)$	N	*VINV*
0.350 00	0.802 54	1	0.802 54
0.700 00	0.475 42	2	0.475 42
1.050 0	0.298 97	3	0.298 97
1.400 0	0.195 16	4	0.195 16
1.750 0	0.130 53	5	0.130 53
2.100 0	0.887 34E-01	6	0.887 34E-01
2.450 0	0.609 87E-01	7	0.609 86E-01
2.800 0	0.422 35E-01	8	0.422 22E-01
3.150 0	0.294 02E-01	9	0.292 91E-01
3.500 0	0.205 43E-01	10	0.198 31E-01
3.850 0	0.143 90E-01	11	0.106 35E-01
4.200 0	0.100 98E-01	12	−0.645 13E-02
4.550 0	0.709 47E-02	13	−0.540 98E-01
4.900 0	0.498 91E-02	14	−0.183 05
5.250 0	0.351 06E-02	15	−0.463 59
7.000 0	0.608 29E-03	20	4.754 3
10.500	0.183 58E-04	30	4.842 9
14.000	0.554 35E-06	40	13.450
16.800	0.337 10E-07	48	2.680 0

other solvable model $v(x)=2(x^{-2}-b^{-2})$, with the parameters $b=17.955$, $c=1.155$ and $N=48$, the same method yields the results that are shown in table 3. Again one notices that the inversion works very well for the first eleven points and then numerical errors become very large.

In the second approach, we start with Thiele's fit of the logarithmic derivative of the wavefunction given by equations (3.6) and (3.15). Since the accumulation of errors in the continued fraction expansion forces us to choose N small and Δ large ($\Delta \simeq 0.35$), in the case of the Eckart potential which varies rapidly as a function of x, we use f_0/f_1 as is given by (3.6) rather than (3.4) as the input. It should be emphasised that the utilisation of (3.6) as the input data differs from the use of the iterative solution of f_0/f_1 mentioned above, since in (3.6) f_0/f_1 is obtained from the exact solution of the differential equation (3.1) at two neighbouring points. In table 4 the ratio of the logarithmic derivative of ψ to $Z_N(\zeta)$ which is calculated from equations (3.4) and (3.6) is given for different values

Table 3. Comparison between the input inverse square potential and *VINV* obtained from the inversion of f_0/f_1. ($b=17.955$, $c=1.155$, $N=48$.)

		$f_N/f_{N+1}=\zeta$	
$X(N)$	$V(N)$	N	*VINV*
1.505 0	0.876 79	1	0.876 79
1.855 0	0.575 02	2	0.575 02
2.205 0	0.405 15	3	0.405 15
2.555 0	0.300 17	4	0.300 17
2.905 0	0.230 79	5	0.230 79
3.255 0	0.182 56	6	0.182 56
3.605 0	0.147 69	7	0.147 69
3.955 0	0.121 66	8	0.121 65
4.305 0	0.101 71	9	0.101 68
4.655 0	0.860 94E-01	10	0.859 97E-01
5.005 0	0.736 36E-01	11	0.738 54E-01
5.355 0	0.635 41E-01	12	0.679 46E-01
5.705 0	0.552 46E-01	13	0.860 24E-01
6.055 0	0.483 47E-01	14	0.201 16
6.405 0	0.425 48E-01	15	0.671 87
8.155 0	0.238 70E-01	20	9.860 0
11.655	0.851 95E-02	30	9.912 3
15.155	0.250 42E-02	40	7.219 4
17.955	−0.102 26E-07	48	−2.019 3

Table 4. The logarithmic derivative of the Eckart wavefunction at the origin obtained from (3.3) divided by $Z_N(\zeta)$ calculated from equations (2.19) and (3.6).

Δ \ k	0.01	0.1	1	5
3.5×10^{-3}	$1.003+10^{-5}$i	$1.003+10^{-4}$i	$1.001+10^{-3}$i	$1-8\times10^{-3}$i
1.75×10^{-2}	$1.017+6\times10^{-5}$i	$1.017+6\times10^{-4}$i	$1.003+5\times10^{-3}$i	$1-4\times10^{-2}$i
0.35×10^{-1}	$1.035+10^{-4}$i	$1.035+1.3\times10^{-3}$i	$1.006+9.7\times10^{-3}$i	$0.997-8.5\times10^{-2}$i
1.75	$1.178+7\times10^{-4}$i	$1.178+7.6\times10^{-3}$i	$1.019+3.7\times10^{-2}$i	$0.937-0.42$i
0.35	$1.36+1.8\times10^{-3}$i	$1.36+1.8\times10^{-2}$i	$1.023+4.7\times10^{-2}$i	$0.74-0.85$i

of k and Δ. As is expected, for small values of Δ, this ratio is very close to unity, but it deviates significantly from this value when both Δ and k become large. In the case of the second model (equation (3.7)), because of the slow variation of the potential we use the exact values of the logarithmic derivative as the input data. The Thiele's fit is obtained by taking 49 points of $Z(k)$ in the range $k=0.1\times10^{-2}$ and $k=45$ and calculating $Z_{48}(\zeta^2-2\zeta)$ according to (4.1). Then by expanding $Z_{48}(\zeta^2-2\zeta)$ as a continued fraction we find the potential $v(x)$. In tables 5 and 6 this method has been applied to the two models of § 3 and different boundary conditions have been used for F_N/F_{N+1}. As the numbers indicate the results of inversion are insensitive to the boundary condition as long as a rational approximation for F_N/F_{N+1} in terms of $\zeta^2-2\zeta$ is used in calculating (2.18). Similar to the results obtained for the direct problem the method is unstable when a large number of points are included in the fit.

6. Discussion

The difference equation (2.7) is not the only possible asymmetric form which is compatible with the rational fraction fit of the logarithmic derivative of the wavefunction. For instance, we can replace $\exp(-\Delta^2 v_n)$ in equation (2.16) by $1-\Delta^2 v_n$ without affecting the basic properties of the equation or its solution. Other possible modifications of this asymmetric difference equation may, in fact, be desirable since the variable $\zeta^2-2\zeta$ occurring in (2.16) does not have a simple physical interpretation. Concerning the numerical accuracy of the results we observe that in this formulation the direct and the inverse problems are solved using the same set of difference equations.

Table 5. Calculation of the Eckart potential from f_0/f_1 when the latter is obtained from Thiele's rational fraction fit to equation (3.6). For comparison the values of the exact potential at these points are given.

		$f_N/f_{N+1}=\zeta$		$f_N/f_{N+1}=1$		$f_N/f_{N+1}=-\frac{1}{2}(\zeta^2-2\zeta)$	
$X(N)$	$V(N)$	N	$VINV$	N	$VINV$	N	$VINV$
0.350 00	0.802 54	1	0.802 60	1	0.802 54	1	0.802 54
0.700 00	0.475 42	2	0.476 20	2	0.475 42	2	0.475 42
1.050 0	0.298 97	3	0.303 62	3	0.298 97	3	0.298 97
1.400 0	0.195 16	4	0.203 10	4	0.195 16	4	0.195 16
1.750 0	0.130 53	5	0.184 53E-01	5	0.130 53	5	0.130 53
2.100 0	0.887 34E-01	6	−1.072 8	6	0.887 35E-01	6	0.887 42E-01
2.450 0	0.609 87E-01	7	−4.317 8	7	0.609 81E-01	7	0.610 84E-01
2.800 0	0.422 35E-01	8	−5.096 1	8	0.421 64E-01	8	0.432 74E-01
3.150 0	0.294 02E-01	9	−1.054 7	9	0.291 41E-01	9	0.389 30E-01
3.500 0	0.205 43E-01	10	2.355 0	10	0.211 44E-01	10	0.948 24E-01
3.850 0	0.143 90E-01	11	13.741	11	0.343 20E-01	11	0.530 72
4.200 0	0.100 98E-01	12	9.824 1	12	0.230 35	12	4.045 0
4.550 0	0.709 47E-02	13	−12.455	13	1.652 1	13	−7.647 1
4.900 0	0.498 91E-02	14	16.272	14	−6.702 8	14	−20.904
5.250 0	0.351 06E-02	15	−3.461 0	15	−14.192	15	−5.671 5
7.000 0	0.608 29E-03	20	−2.410 3	20	2.127 4	20	−10.595
10.500	0.183 58E-04	30	−4.940 3	30	4.459 9	30	3.320 6
14.000	0.554 35E-06	40	−10.848	40	−8.495 6	40	−8.296 4
16.800	0.337 10E-07	48	−3.314 8	48	−2.152 9	48	−2.396 7

Table 6. The result of the inversion of f_0/f_1 for the inverse square potential using Thiele's fit of equation (3.15).

		$f_N/f_{N+1}=\zeta$		$f_N/f_{N+1}=1$		$f_N/f_{N+1}=-\frac{1}{2}(\zeta^2-2\zeta)$	
$X(N)$	$V(N)$	N	$VINV$	N	$VINV$	N	$VINV$
1.505 0	0.876 79	1	0.876 79	1	0.876 79	1	0.876 79
1.855 0	0.575 02	2	0.575 02	2	0.575 02	2	0.575 02
2.205 0	0.405 15	3	0.405 28	3	0.405 15	3	0.405 15
2.555 0	0.300 17	4	0.301 33	4	0.300 17	4	0.300 17
2.905 0	0.230 79	5	0.237 19	5	0.230 79	5	0.230 79
3.255 0	0.182 56	6	0.206 08	6	0.182 57	6	0.182 57
3.605 0	0.147 69	7	0.205 09	7	0.147 74	7	0.147 69
3.955 0	0.121 66	8	0.200 36	8	0.121 80	8	0.121 54
4.305 0	0.101 71	9	0.938 84E-01	9	0.101 63	9	0.994 09E-01
4.655 0	0.860 94E-01	10	−0.858 60E-01	10	0.752 60E-01	10	0.582 41E-01
5.005 0	0.736 36E-01	11	1.283 8	11	−0.758 32E-01	11	−0.177 81
5.3550	0.635 41E-01	12	19.023	12	−1.2359	12	−1.646 6
5.7050	0.552 46E-01	13	−18.965	13	−6.160 5	13	−6.628 6
6.0550	0.483 47E-01	14	8.315 8	14	−10.329	14	−9.348 4
6.4050	0.425 48E-01	15	−2.229 2	15	−4.246 2	15	−2.501 6
8.1550	0.238 70E-01	20	25.205	20	−2.885 8	20	−2.608 8
11.655	0.851 95E-02	30	−14.002	30	11.028	30	25.837
15.155	0.250 42E-02	40	−5.096 8	40	−7.428 5	40	−9.183 3
17.955	−0.102 26E-07	48	−2.053 5	48	−2.744 5	48	−2.273 6

While the results for the direct problem can be found with great accuracy by choosing N to be large (table 1), in the inverse problem the numerical errors accumulate and this limits the choice of N. We have studied this by trying different but algebraically equivalent forms of computing the continued fraction (Baker 1975) and found that the accuracy changes significantly with the form used and the number of arithmetic operations involved in the calculation. Let us now briefly mention the error estimates for the difference equation (2.7). In the direct problem the error due to the rational approximation of the boundary condition (2.20) is not magnified, but the error due to roundings in arithmetical operation in a single step is increased by a factor N (Blanch 1964). For the inverse problem the error due to the finite-difference approximation for the logarithmic derivative (2.19) is not as important as the round off errors in the J-fraction expansion. For the two models that we have studied these errors seem to be independent of the shape and the strength of the potential. Once a more accurate numerical technique for obtaining the continued fraction expansion of the Padé approximant is found, then it may be possible to apply this method to a number of interesting problems including the following.

(i) Inverse scattering problem for static potentials plus a boundary condition model at short distances. As is well known the concept of the nucleon–nucleon potential breaks down for very short distances (less than 0.5 F), (see, for instance, Moravcsik 1972), and it is reasonable to represent the interaction in the innermost region by a boundary condition which may or may not be energy dependent. Since in boundary condition models the logarithmic derivative is given, one may conjecture that a procedure similar to what has been discussed in this paper can be used to determine the outer potential from the scattering phaseshifts.

(ii) Complex potentials. The present formulation allows for the direct or the inverse problems when the interaction is complex. Since a part of the problem of instability of our numerical computation is due to the rapid growth of the imaginary part of $\exp(-\Delta^2 v_n)$ when the number of points increases, therefore in inverting R matrices corresponding to the complex optical potentials, we expect even more numerical instability than the present case.

(iii) Wave propagation in an inhomogeneous medium. By a simple modification, i.e. using travel time coordinates (Ware and Aki 1968), the same method can be used for the inversion of the problem of one-dimensional wave propagation.

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