The recursion method of a linear operator inversion. III

1983 J. Phys. A: Math. Gen. 16 3313

(http://iopscience.iop.org/0305-4470/16/14/022)

J. Phys. A: Math. Gen. 16 (1983) 3313–3323. Printed in Great Britain

The recursion method of a linear operator inversion: III

M Znojil
Institute of Nuclear Physics, Czechoslovak Academy of Sciences, 250 67 Řež, Czechoslovakia

Received 15 February 1983

Abstract. We suggest constructing an inverse of the infinite-dimensional matrix Q by means of its recurrent algebraic decomposition into the easily invertible two-diagonal factors. The merits and feasibility of the method are illustrated on the five-diagonal matrices. Quartic and decadic–decadic anharmonic propagators are chosen as examples of the application.

1. Introduction

In quantum mechanics, manipulations with matrices (Hamiltonians, transition operators, etc) are usually facilitated by their diagonalisation. Limitations of this technique may be both computational and interpretational in character. As a consequence, the direct use of the next, tridiagonal form of matrices is also quite frequent and may affect both the approximation schemes (Bassichis and Strayer 1978 etc) and the construction of models (e.g. Haydock and Kelly 1975).

In the former context, one of the important characteristics of the infinite tridiagonal matrices is their easy invertibility in terms of continued fractions (Wall 1948). In paper I of the present series (Znojil 1976) we have, therefore, weakened the tridiagonality restriction and succeeded in inverting algebraically even the general Hessenberg matrix Q_{ij} (which is zero for all $j \geqslant i+2$) in terms of the auxiliary 'extended continued fractional' (ECF) sequence f_k. These ECF quantities were defined by the recurrences

$$f_k(N) = \left(a_k^{(1)} + \sum_{j=2}^{N-k+1} a_k^{(j)} \prod_{i=1}^{j-1} f_{k+i}(N) \right)^{-1}$$
$$k = 1, 2, \ldots, N \qquad f_{N+1}(N) = f_{N+2}(N) = \ldots = 0 \tag{1.1}$$

in the limit $N \to \infty$ ($f_k = \lim_{N\to\infty} f_k(N)$), i.e. totally analogous with the classical continued fractions.

In paper II (Znojil 1978) we used the generalised (matrix) form of recurrences (1.1) to invert any sparse matrix Q by means of its Hessenberg-type partitioning. In this paper, we intend to suggest an alternative generalisation of I which will be based on a representation of Q in the form of a product of the two-diagonal matrices.

For the sake of brevity, we consider in detail only the simplest non-trivial case, namely the matrix Q given in the five-diagonal form. Thus, the method is presented in § 2, while in § 3 the convergence and its acceleration are discussed thoroughly in the ECF context. Finally, § 4 is devoted to physical examples (anharmonic propagators), and the various possible generalisations of the formalism are reviewed in § 5.

2. The method

2.1. Five-diagonal matrices

Any finite five-diagonal matrix Q

$$\begin{pmatrix} Q_{11} & Q_{12} & Q_{13} & 0 & \dots & & & & & & 0 \\ \dots \\ 0 & \dots & 0 & Q_{kk-2} & Q_{kk-1} & Q_{kk} & Q_{kk+1} & Q_{kk+2} & 0 & \dots & 0 \\ \dots \\ 0 & \dots & & & & & 0 & Q_{NN-2} & Q_{NN-1} & Q_{NN} \end{pmatrix} \quad (2.1)$$

may be inverted numerically by the algorithms described by Grund (1977). Alternatively, it may also be partitioned (into the blockwise tridiagonal form) and inverted in terms of the (2×2)-dimensional matrix continued fractions (MCF) (Znojil 1977).

In this paper, we intend to construct Q^{-1} algebraically, by means of its complete factorisation into the easily invertible two-diagonal matrices

$$\begin{pmatrix} 1 & \alpha_1 & & \\ & 1 & \alpha_2 & \\ & & \ddots & \ddots \end{pmatrix} = \begin{pmatrix} 1 & -\alpha_1 & \alpha_1\alpha_2 & -\alpha_1\alpha_2\alpha_3 & \dots \\ & 1 & -\alpha_2 & \alpha_2\alpha_3 & \dots \\ & & \dots \end{pmatrix}^{-1}. \quad (2.2)$$

In the 'non-degenerate' cases with $Q_{k-2k} \neq 0$ and $Q_{kk+2} \neq 0$, we shall write

$$Q = \begin{pmatrix} G_1 & & \\ & \ddots & \\ & & G_N \end{pmatrix} \times H \times \begin{pmatrix} D_1 & & \\ & \ddots & \\ & & D_N \end{pmatrix}$$

$$H = \begin{pmatrix} a_1 & b_1 & 1 & \dots \\ \dots \\ \dots & 1 & c_k & a_k & b_k & 1 & \dots \\ \dots \\ \dots & & & & 1 & c_N & a_N \end{pmatrix} \quad (2.3)$$

$$Q_{kk-2} = G_k D_{k-2} \qquad Q_{kk+2} = G_k D_{k+2}$$

with the trivial recurrences defining

$$\begin{aligned} D_3 &= Q_{13}/G_1 \qquad & D_4 &= Q_{24}/G_2 \dots \\ G_3 &= Q_{31}/D_1 \qquad & G_4 &= Q_{42}/D_2 \dots \end{aligned} \quad (2.4)$$

from the first four free values G_1, G_2, D_1 and D_2. This simplifies the further notation—we may put

$$H = \begin{pmatrix} 1 & \alpha_1 & & \\ & \ddots & \ddots & \\ & & 1 & \alpha_{N-1} \\ & & & 1 \end{pmatrix} \times \begin{pmatrix} 1 & \beta_1 & & \\ & \ddots & \ddots & \\ & & 1 & \beta_{N-1} \\ & & & 1 \end{pmatrix} \times \begin{pmatrix} 1/f_1 & & & \\ & \ddots & & \\ & & 1/f_{N-1} & \\ & & & 1/f_N \end{pmatrix}$$

$$\times \begin{pmatrix} 1 & & & \\ \gamma_2 & 1 & & \\ & \ddots & \ddots & \\ & & \gamma_N & 1 \end{pmatrix} \times \begin{pmatrix} 1 & & & \\ \delta_2 & 1 & & \\ & \ddots & \ddots & \\ & & \delta_N & 1 \end{pmatrix} \quad (2.5)$$

and obtain the required result in the form

$$Q^{-1}=\begin{pmatrix} D_1^{-1} & & \\ & \cdot & \\ & & D_N^{-1}\end{pmatrix}\times H^{-1}\times\begin{pmatrix} G_1^{-1} & & \\ & \cdot & \\ & & G_N^{-1}\end{pmatrix} \tag{2.6}$$

$$H^{-1}=\begin{pmatrix} 1 & & \\ -\delta_2 & 1 & \\ \delta_2\delta_3 & -\delta_3 & 1 \\ & \cdots & \end{pmatrix}\times\begin{pmatrix} 1 & & \\ -\gamma_2 & 1 & \\ \gamma_2\gamma_3 & -\gamma_3 & 1 \\ & \cdots & \end{pmatrix}\times\begin{pmatrix} f_1 & & \\ & f_2 & \\ & & \ddots \end{pmatrix}$$

$$\times\begin{pmatrix} 1 & -\beta_1 & \beta_1\beta_2 & \cdots \\ & 1 & -\beta_2 & \cdots \\ & & \cdots & \end{pmatrix}\times\begin{pmatrix} 1 & -\alpha_1 & \alpha_1\alpha_2 & \cdots \\ & 1 & -\alpha_2 & \cdots \\ & & \cdots & \end{pmatrix}.$$

In this way, the problem of inversion becomes reduced to the problem of the algebraic factorisation (2.5).

2.2. *Recurrent factorisation*

In (2.5), the $2(N-2)$ elements of the two outer (unit) diagonals of H are represented by the products

$$1=\alpha_k\beta_{k+1}/f_{k+2} \qquad 1=\delta_{k+1}\gamma_{k+2}/f_{k+2} \qquad k=1,2,\ldots,N-2. \tag{2.7}$$

When we denote $u_k=\alpha_k+\beta_k$ and $v_{k+1}=\gamma_{k+1}+\delta_{k+1}$, we may re-express also the $2(N-1)$ elements b_k and c_{k+1} of H in the form

$$\begin{aligned} b_k &= u_k/f_{k+1}+\alpha_k\beta_{k+1}v_{k+2}/f_{k+2} \\ c_{k+1} &= v_{k+1}/f_{k+1}+u_{k+1}\delta_{k+1}\gamma_{k+2}/f_{k+2} \qquad k=1,2,\ldots,N-1. \end{aligned} \tag{2.8}$$

Finally, the main diagonal of H is related to the right-hand side of (2.5) by the relations

$$a_k=\frac{1}{f_k}+\frac{u_kv_{k+1}}{f_{k+1}}+\frac{\alpha_k\beta_{k+1}\delta_{k+1}\gamma_{k+2}}{f_{k+2}} \qquad k=1,2,\ldots,N-1. \tag{2.9}$$

Since $b_N=\alpha_N=\beta_N=0$ and $c_{N+1}=\gamma_{N+1}=\delta_{N+1}=0$, we may initialise the recurrences (2.7) by any $\alpha_{N-1}(=u_{N-1}-\beta_{N-1})$ and $\delta_N(=v_N-\gamma_N)$ and define all the four two-diagonal factors in (2.5) by the recurrences

$$\alpha_k=f_{k+2}/(u_{k+1}-\alpha_{k+1}) \qquad \delta_{k+1}=f_{k+2}/(v_{k+2}-\delta_{k+2}) \qquad k=1,2,\ldots,N-2. \tag{2.10}$$

Similarly, the fundamental sequences u_k, v_{k+1} and $1/f_{k+2}$, $k=1,2,\ldots,N-1$, $(1/f_{N+1}=0)$ may be generated from the trivial initialisation

$$u_N=v_{N+1}=f_{N+1}=0 \qquad f_N=1/a_N. \tag{2.11}$$

The corresponding recurrences

$$u_k=f_{k+1}(b_k-v_{k+2}) \qquad v_{k+1}=f_{k+1}(c_{k+1}-u_{k+1}) \tag{2.12}$$

and

$$f_k=1/(a_k-u_kv_{k+1}/f_{k+1}-f_{k+2}) \qquad k=N-1,N-2,\ldots,1 \tag{2.13}$$

are coupled and follow from (2.8) and (2.9), respectively. This completes our description of the numerical recurrent algorithm. We have only to perform the multiplication in (2.6),

$$H^{-1}=\begin{pmatrix} f_1, & -(\alpha_1+\beta_1)f_1, & (\alpha_1\alpha_2+\beta_1\beta_2+\beta_1\alpha_2)f_1, & \dots \\ -(\gamma_2+\delta_2), & (\alpha_1+\beta_1)(\alpha_2+\beta_2)f_1+f_2, & \dots & \\ \dots & & & \end{pmatrix} \tag{2.14}$$

and obtain the inverse matrix for any finite $N<\infty$.

Let us note that the algorithm has the following two merits.

(1) Inverses of the lower submatrices of H

$$H_{[M]}=\begin{pmatrix} a_M & b_M & 1 & \dots & \\ \dots & & & & \\ \dots & & 1 & c_N & a_N \end{pmatrix} \tag{2.15}$$

are obtainable, by a mere change of indices

$$H_{[M]}^{-1}=\begin{pmatrix} 1 & & \\ -\delta_{M+1} & 1 & \\ \dots & & \\ \dots & & 1 \end{pmatrix}\times\dots\times\begin{pmatrix} 1 & -\alpha_M & & \dots \\ & 1 & -\alpha_{M+1} & \dots \\ & & \dots & \\ & & \dots & 1 \end{pmatrix}, \tag{2.16}$$

as byproducts of our recurrent procedure. This may prove to be useful in the applications of the type described in § 4 below.

(2) The upper submatrices of the inverse H^{-1} have a simple form (2.14) where α, β, γ and δ may systematically be replaced by u and v only,

$$H^{-1}=\begin{pmatrix} f_1, & -u_1f_1, & (u_1, u_2-f_3)f_1, & \dots \\ -v_2f_1, & (a_1-f_3)f_2f_1, & (a_1b_2+c_2-a_1u_3)f_2f_2f_3, & \dots \\ \dots & & & \end{pmatrix} \tag{2.17}$$

(see appendix for details).

2.3. *The $N\to\infty$ limit*

Provided that the sequences u_k, v_{k+1} and f_{k+2} are known in the infinite-dimensional limit $N\to\infty$, the values of α_k or δ_{k+1} are given by their respective analytic continued fractional expansions

$$\alpha_k=\cfrac{f_{k+2}}{u_{k+1}-\cfrac{f_{k+3}}{u_{k+2}-\dots}} \qquad \delta_{k+1}=\cfrac{f_{k+2}}{v_{k+2}-\cfrac{f_{k+3}}{v_{k+3}-\dots}}. \tag{2.18}$$

In the light of the definitions of u_k and v_{k+1} we may write also, alternatively,

$$\beta_k=u_k-\cfrac{f_{k+2}}{u_{k+1}-\cfrac{f_{k+3}}{u_{k+2}-\dots}} \qquad \gamma_{k+1}=v_{k+1}-\cfrac{f_{k+2}}{v_{k+2}-\cfrac{f_{k+3}}{v_{k+3}-\dots}} \tag{2.19}$$

and apply the standard convergence criteria (Wall 1948).

In a similar way, sequences u_k and v_{k+1} may be defined directly in terms of the only sequence f_k

$$\begin{aligned} u_k &= f_{k+1}b_k - f_{k+1}f_{k+2}c_{k+2} + f_{k+1}f_{k+2}f_{k+3}b_{k+2} - \dots \\ v_{k+1} &= f_{k+1}c_{k+1} - f_{k+1}f_{k+2}b_{k+1} + f_{k+1}f_{k+2}f_{k+3}c_{k+3} - \dots \end{aligned} \tag{2.20}$$

(see (2.12)). The appropriate convergence criteria should be used again (e.g. Korn and Korn 1968).

In the third step, the recurrence (2.13) may be reformulated in a surprising analogy with I.

Theorem. The diagonal matrix elements $1/f_k$ in (2.5) coincide with the ECF quantities of the form (1.1).

Proof. We may consider only $k = 1$ and $N = \infty$ without loss of generality. Then, to obtain the expansion of f_1 ($=H_{11}^{-1}$, cf (2.14)), we have to employ (2.13) with $k = 2$ as a redefinition of

$$f_3 = -f_2f_3f_4 + a_2f_2f_3 - u_2f_2v_3$$

and insert it into (2.13) with $k = 1$. After an easy rearrangement (cf (2.12) with $k = 1$ and (2.20)), we get precisely formula (1.1) where $k = 1$ and the compact prescription

$$\begin{aligned} &a_1^{(1)} = a_1 \qquad a_1^{(2)} = -b_1c_2 \qquad a_1^{(3)} = b_1b_2 + c_2c_3 - a_2 \\ &a_1^{(4)} = -b_1c_4 - c_2b_3 + 1 \qquad a_1^{(2n-1)} = b_1b_{2n-2} + c_2c_{2n-1} \\ &a_1^{(2n)} = -b_1c_{2n} - c_2b_{2n-1} \qquad n \geq 3 \end{aligned} \tag{2.21}$$

defines the coefficients.

In the final step, the matrix elements of H^{-1} are to be specified as the sums of products of the ECF quantities f_k (further algebra is done in the appendix).

3. Fixed point initialisations

3.1. *Ambiguities of the inversion*

In the infinite-dimensional cases, we may construct the non-trivial solutions $w_k = -w_{k-1}/\alpha_{k-1}$, $k = 2, 3, \dots$ to the homogeneous systems of equations

$$\begin{pmatrix} 1 & \alpha_1 & & \\ & 1 & \alpha_2 & \\ & & \ddots & \ddots \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \\ \vdots \end{pmatrix} = 0 \tag{3.1}$$

which can even be normalised for $|\alpha_k| \geq 1 + \varepsilon$, $\varepsilon > 0$, $k > k_0$. Therefore, up to some exceptional situations where $w_1 \neq 0$ (Znojil 1983) we must complement (2.2) by the condition $w_1 (= w_2 = \dots) = 0$.

Furthermore, the different formal inverses H^{-1} may also be generated by the various auxiliary sequences, i.e. by the *a priori* unrestricted free choice of the four initial values

$$u_M \qquad v_{M+1} \qquad f_{M+1} \qquad f_{M+2} \tag{3.2}$$

at some fixed $M \geqslant 1$. Hence, the choice of the values (3.2) represents, in fact, an independent 'boundary-condition-type' requirement. It has to suppress completely the algebraic ambiguity of the formal inverse (2.6) with $N = \infty$.

In general, this need not necessarily be equivalent to (2.11) in the limit $N \to \infty$ but we accept such a specification of H^{-1} and intend only to accelerate the $N \to \infty$ convergence by appropriate modifications of (2.11).

3.2. *Fixed point approximation*

At any finite index $k = M < \infty$, merely one of the initialisations (3.2) may be precisely equivalent to the $N \to \infty$ limit of (2.11). In its vicinity, there still exists a class of the approximate or 'effective' initialisations which would give the exact result in the $M \to \infty$ limit. Finally, in the light of the example given in § 4.2 some of the remaining initialisations may generate, in principle, entirely non-physical inverse matrices.

In practical applications, a construction of the 'effective' initialisation may often be based on the weak N-dependence of the approximate values (3.2) when evaluated from (2.11) with some finite $N \gg M$. Usually, the reliability of such a construction is closely related to the asymptotic smoothness (i.e. slowness of variation or non-oscillatory character) of the elements $c_M \sim c$, $b_M \sim b$ and $a_M \sim a$ of H as functions of their index $M \gg 1$.

Vice versa, in the smooth cases we may also expect an approximate index-independence of the asymptotic auxiliary sequences (3.2) themselves. Obviously, the constant approximants

$$f_M \sim f \qquad u_M \sim u \qquad v_{M+1} \sim v \qquad \alpha_M \sim \alpha \qquad \delta_{M+1} \sim \delta \ldots$$

must satisfy the approximate recurrences and may be therefore identified with some of the roots of the system

$$\begin{aligned} &\alpha^2 - \alpha u + f = 0 \qquad \delta^2 - \delta v + f = 0 \\ &u = (b - v)f \qquad v = (c - u)f \\ &1/f = a - (uv/f) - f \end{aligned} \tag{3.3}$$

i.e. with the stationary (fixed) points of the five mappings (2.10)–(2.13).

The algebraic determination of the fixed points may be reduced here to the four definitions

$$\begin{aligned} 2\alpha &= u + (u^2 - 4f)^{1/2} \qquad 2\gamma = v + (v^2 - 4f)^{1/2} \\ 2\beta &= u - (u^2 - 4f)^{1/2} \qquad 2\delta = v - (v^2 - 4f)^{1/2} \end{aligned} \tag{3.4}$$

of the asymptotic two-diagonal factors in (2.5), with

$$\begin{aligned} &u = \frac{f}{1+f} B + \frac{f}{1-f} A \qquad v = \frac{f}{1+f} B - \frac{f}{1-f} A \\ &B = (b + c)/2 \qquad A = (b - c)/2 \end{aligned} \tag{3.5}$$

and accompanied by the last item of (3.3). When we denote

$$2X = f + 1/f \qquad \text{or} \qquad f = X - (X^2 - 1)^{1/2}$$

for simplicity, this equation appears to be a cubic one,

$$2X = a - B^2/(2X+2) + A^2/(2X-2) \tag{3.6}$$

and defines the last unknown fixed-point parameter in a purely algebraic manner.

The solution of (3.6) is not unique. Examples of analysis of the corresponding 'boundary-type' conditions may be found in I or in § 4.2.

3.3. A systematic acceleration of convergence

For the matrices H which violate the smoothness requirement, we have to reintroduce the indices into the definitions (3.4)–(3.6) ($a \to a_M$, B, $A \to (b_M \pm c_{M+1})/2$ and $X \to X(M+1)$ in (3.6), $f \to f(M+1)$ in (3.5) and $u \to u(M)$, $v \to v(M+1)$, $\alpha, \beta \to \alpha(M)$, $\beta(M)$ and $\gamma, \delta \to \gamma(M+1)$, $\delta(M+1)$ in (3.4)) and consider the deviations

$$U_k = u_k - u(k) \qquad V_{k+1} = v_{k+1} - v(k+1) \qquad F_{k+1} = f_{k+1} - f(k+1) \tag{3.7}$$

etc, as the new auxiliary sequences. For them, the new recurrences may be derived by simple insertions.

On the basis of the weakened 'smoothness' assumption, we may again introduce the fixed point approximation

$$U_k \sim U(k) \qquad V_{k+1} \sim V(k+1) \qquad F_{k+1} \sim F(k+1)$$

etc. Its merit is an expected smallness of the roots—we may specify them uniquely from the linearised equations giving, for example, $F(k+1)$ as a simple rational function of the quantities f, f^Δ, S^2, T^2 and S^Δ where

$$f^\Delta = f(k+1) - f(k+2)$$

$$u(k) = S + T \qquad v(k+1) = S - T$$

$$u^\Delta = u(k) - u(k+1) = S^\Delta + T^\Delta$$

$$v^\Delta = v(k+1) - v(k+2) = S^\Delta - T^\Delta.$$

In principle, the higher-order fixed-point approximants may be generated algebraically in a systematic way. Their shortcoming is their increasingly complicated form—for example, we get (with $\varphi = f(k+1) + F(k+1)$)

$$U(k) = \frac{F(k+1)}{f(k+1)}\left(\frac{S}{1+\varphi} + \frac{T}{1-\varphi}\right) + \varphi\left(\frac{S^\Delta}{1+\varphi} - \frac{T^\Delta}{1-\varphi}\right)$$

as the second-order analogue of (3.5), the sixth-order polynomial counterpart to (3.6), etc.

4. Applications

4.1. Anharmonic oscillator

In the harmonic oscillator basis $|n\rangle$, $n = 0, 1, \ldots$, some properties of bound states ψ of the anharmonic Hamiltonian

$$\mathcal{H} = p^2 + x^2 + \lambda x^4$$

may be inferred directly from the Schrödinger equation

$$\mathcal{H}\psi = E\psi$$

or rather from its projection

$$\hat{q}Q\psi = 0 \qquad Q = E - \hat{q}\mathcal{H}\hat{q} \qquad \hat{q} = \hat{q}^2$$

i.e. from the linear relations

$$Q\chi = \varphi \qquad \chi = \hat{q}\psi \qquad \varphi = \hat{q}\mathcal{H}\hat{p}\cdot\hat{p}\psi \tag{4.1}$$

between the 'model-space' projections $\hat{p}\psi$ ($\hat{p} = 1 - \hat{q} = \Sigma_{m=0}^{n} |m\rangle\langle m|$) and the rest of ψ. The main reason is that the matrix Q is five-diagonal; an explicit form of its matrix elements may be found, e.g., in Graffi and Grecchi (1975).

The explicit inversion of Q in (4.1) may be based on its factorisation (2.5) in the asymptotic region where we may put

$$G_i = D_i = n^2 \times \text{constant}(i) \times \mathrm{O}(n) \qquad n \gg 1$$

and

$$a_i = a = 6 \qquad b_i = c_{i+1} = b = B = 4 \qquad A = 0$$

in (2.3). Then, the fixed-point prescription (3.6) degenerates to the quadratic equation with the unique root $X = f = 1$. From the remaining relations, we get also $u = v = 2$, $\alpha = \beta = \gamma = \delta = 1$ and

$$H^{-1} = \begin{pmatrix} 1 & -2 & 3 & -4 & \dots \\ -2 & 5 & -8 & 11 & \dots \\ 3 & -8 & 14 & -20 & \dots \\ \dots & & & & \end{pmatrix} \tag{4.2}$$

(cf (2.6)). Hence, in the leading order approximation, the algebraic inversion of Q is simple and unique. It also demonstrates that the convergence of $\|\psi\|$, if any, is rather slow and may be characterised only in terms of the higher-order corrections. This will not be done here.

4.2. Decadic—decadic propagator

A symmetrically anharmonic phenomenological Hamiltonian

$$\mathcal{H} = \alpha_5 p^{10} + \alpha_4 p^8 + \dots + \alpha_1 p^2 + \beta_1 x^2 + \dots + \beta_4 x^8 + \beta_5 x^{10} \qquad \alpha_5 > 0 \qquad \beta_5 > 0 \tag{4.3}$$

was introduced by Znojil (1981). In the asymptotic ($\hat{q}$-projected, high-lying harmonic-oscillator) region, it was shown to acquire approximately the five-diagonal form, with

$$G_i = D_i = n^5 \times \text{constant}(i) + \mathrm{O}(n^4)$$

$$a_i = a = 25.2 \qquad b_i = c_{i+1} = B = 12 \qquad A = 0$$

in (2.3). The numerical inversion of H gave $H_{11}^{-1} = 0.055\,728\dots$.

In the present ECF context, we shall reproduce this numerical value by purely non-numerical means, clarify its algebraic background and illustrate the character of ambiguities met during its derivation. To achieve this, it is sufficient to apply the results of § 3—the two roots of (3.6) and four values of f are listed in table 1.

Table 1. Numerical values of parameters for the asymptotic factorisation of the decadic–decadic propagators ($R_{\pm} = 1 \pm 2/\sqrt{5}$, second row is not spurious).

X	$f(=H_{11}^{-1})$	u	$\max(\gamma, \delta)$	$\min(\gamma, \delta)$
9	$5R_+^2(=17.944\,271\,90\ldots)$	$6R_+$	$5R_+(=19.47\ldots)$	R_+
9	$5R_-^2(=0.055\,728\,090\ldots)$	$6R_-$	$5R_-(=0.527\ldots)$	R_-
$\frac{13}{5}$	5	10	$5R_+$	$5R_-$
$\frac{13}{5}$	$\frac{1}{5}$	2	$R_-(=1.894\ldots)$	R_-

The second row in table 1 reproduces the numerical solution and coincides, therefore, with the stable fixed point of the corresponding mappings initialised by (2.11) at $N \to \infty$. The remaining items define the spurious solutions and the inverse H^{-1} which cannot be obtained by the ordinary truncation method.

Without any recourse to numerical computations, the rigorous elimination of the spurious inverses is easy in the present example. Indeed, we get the wavefunction $\hat{q}\psi$ from (4.1) and (4.3) as a superposition of the first $n+1$ columns of the matrix

$$\begin{pmatrix} 1 & & \\ -\delta & 1 & \\ \delta^2 & -\delta & 1 \\ & \ldots & \end{pmatrix} \times \begin{pmatrix} 1 & & \\ -\gamma & 1 & \\ \gamma^2 & -\gamma & 1 \\ & \ldots & \end{pmatrix} = \begin{pmatrix} 1 & & \\ -(\gamma+\delta) & 1 & \\ \gamma^2+\gamma\delta+\delta^2 & -(\gamma+\delta) & 1 \\ \ldots & & \end{pmatrix}. \tag{4.4}$$

Since

$$\delta^m + \delta^{m-1}\gamma + \ldots + \gamma^m = (\delta^{m+1} - \gamma^{m+1})/(\delta - \gamma) \qquad \delta \neq \gamma \tag{4.5}$$

we arrive at the rigorous asymptotic estimate

$$|\langle m+1|\chi\rangle/\langle m|\chi\rangle| = \max(|\delta|, |\gamma|) \qquad m \gg n \geqslant 0. \tag{4.6}$$

Now, the geometric convergence criterion (Korn and Korn 1968) implies that none of the spurious fixed points f can lead to the normalisable eigenstate ψ or χ of the decadic–decadic Hamiltonian $\mathscr{H}$ since $\max(\gamma, \delta) > 1$.

5. Generalisations and summary

Any band matrix Q with t upper and s lower diagonals may be factorised in analogy with the $t = s = 2$ example of § 2. Similarly, even to invert any blockwise Hessenberg matrix with the variable partitions, the same decomposition into the two-diagonal matrix factors with some zero elements $\alpha_i, \ldots$ may be used. The resulting inverses will be generalisations of equation (2.6).

A peculiarity of the three-and five-diagonal examples lies in their non-numerical character (cf our ECF theorem, the formulae in the appendix or the simplicity of the fixed points). In the applications, they may therefore be used as the solvable models of interaction (see our first example) etc.

The pentadiagonal extension of the tridiagonal matrices may also prove to be useful as the mathematical approximant whenever the ordinary methods diverge (cf, e.g., the perturbative expansion of our first example as discussed, e.g., by Killingbeck

(1977)), or oscillate ('averages' of Richardson and Blankenbecler (1979) resemble our fixed points). In numerical practice, they could also sometimes replace the standard (finite-submatrix) truncation approximants in a way similar to our second example.

Appendix. Compactified form of inverse of the five-diagonal matrix H

The explicit form (2.6) of H^{-1} contains the four sequences α_k, β_k, γ_{k+1} and δ_{k+1}. The main idea of their replacement by mere 'sums' u_k and v_{k+1} (compare equations (2.14) and (2.17)) lies in the direct use of the 'upper times lower' decomposition (2.5) written in the form

$$H=\begin{pmatrix}1 & u_1 & f_3 & & \\ & 1 & u_2 & f_4 & \\ & & \dots & & \\ & & & 1 & u_{N-1}\\ & & & & 1\end{pmatrix}\times\begin{pmatrix}1/f_1 & & \\ & \ddots & \\ & & 1/f_N\end{pmatrix}\times\begin{pmatrix}1 & & & \\ v_2 & 1 & & \\ f_3 & v_3 & 1 & \\ & \dots & & \\ \dots & f_N & v_N & 1\end{pmatrix}. \tag{A1}$$

We shall now construct H^{-1} by inverting the triangular factors in (A1),

$$H^{-1}=\begin{pmatrix}1 & & & \\ z_2^{(1)} & 1 & & \\ z_3^{(1)} & z_2^{(2)} & 1 & \\ \dots & & & \\ z_N^{(1)} & \dots & & 1\end{pmatrix}\times\begin{pmatrix}f_1 & & & \\ & f_2 & & \\ & & \ddots & \\ & & & f_N\end{pmatrix}\times\begin{pmatrix}1 & y_1^{(1)} & y_2^{(1)} & \dots & y_{N-1}^{(1)}\\ & 1 & y_1^{(2)} & \dots & y_{N-2}^{(2)}\\ & & \ddots & \dots & \\ & & & & 1\end{pmatrix}. \tag{A2}$$

Such an approach cannot be generalised too easily but it gives a more compact result—the multiplication in (A2) is still feasible 'by hand' for the five-diagonal H. We intend to show here how the necessary algebraic manipulations may employ the recurrences valid for the sequences u_k, v_{k+1} and f_k.

Without loss of generality, we shall evaluate only the sequence $z_k^{(1)}$, $k=2,3,\dots N$. From its definition we get, omitting the upper indices,

$$v_2+z_2=0 \qquad f_3+v_3z_2+z_3=0\dots$$

i.e. with $z_1=1$ and $z_0=0$,

$$z_k=-v_kz_{k-1}-f_kz_{k-2} \qquad k=2,3,\dots,N. \tag{A3}$$

The explicit form of the first few expressions z_k inspires us to use the ansatz

$$\begin{gathered}z_k=f_2f_3\dots f_k[A_k+f_{k+1}(B_k+D_kv_{k+2})]\\ A_1=-D_2=1 \qquad B_1=D_1=0 \qquad A_2=-c_2 \qquad B_2=b_2\dots.\end{gathered} \tag{A4}$$

In this setting, the mathematical induction is easy (cf also the proof of the theorem in § 2) and gives the recurrences

$$\begin{gathered}D_k=-A_{k-1} \qquad B_k=A_{k-2}+A_{k-1}b_k\\ A_k=-(B_{k-2}+a_{k-1}A_{k-2}+c_kA_{k-1}) \qquad k=3,4,\dots.\end{gathered} \tag{A5}$$

Obviously, the first two of them are mere definitions while the third one,

$$A_k=-(c_kA_{k-1}+a_{k-1}A_{k-2}+b_{k-2}A_{k-3}+A_{k-4}), \tag{A6}$$

has an explicit solution

$$A_k = (-1)^{k+1} \det S(k) \qquad k = 2, 3, \ldots, N$$

$$S(k) = \begin{pmatrix} c_1 & a_2 & b_2 & 1 & 0 & \ldots & \\ 1 & c_3 & a_3 & b_3 & 1 & 0 & \ldots \\ & \ldots & & & & & \\ 0 & \ldots & & 0 & 1 & c_{k-1} & a_{k-1} \\ 0 & \ldots & & & 0 & 1 & c_k \end{pmatrix}. \tag{A7}$$

After a simple rearrangement of (A4), we get the final formula

$$z_k^{(1)} = (-1)^{k+1} f_2 f_3 \ldots f_k [\det S(k) - u_k \det S(k-1) + f_{k+1} \det S(k-2)]$$
$$k = 2, 3, \ldots, N \qquad \det S(0) = 0 \qquad \det S(1) = 1. \tag{A8}$$

Its main merits are:

(i) When inserted into (A2), it provides a compact definition of H_{ij}^{-1} for the small indices $i \neq j \ll N$.

(ii) Due to its linear u-dependence (which simplifies also the transpositions $H(u, v) = H^{\mathrm{T}}(v, u)$), its ECF representation is very similar to the ECF denominator itself.

(iii) The presence of factors $f_i f_{i+1} \ldots f_{i+k}$ in H_{ii+k}^{-1} resembles and generalises the continued-fractional factorisation encountered in the tridiagonal case (see I) and may also be generalised to the more-diagonal matrices.

The diagonal matrix elements H_{ii}^{-1} are exceptional. Their ECF form is extremely simple

$$H_{ii}^{-1} = f_1 f_2 \ldots f_i [\det H(i-1) - f_{i+1} \det H(i-2)]$$
$$i = 1, 2, \ldots \qquad \det H(-1) = 0 \qquad \det H(0) = 1 \tag{A9}$$
$$H(i) = \begin{pmatrix} a_1 & b_1 & 1 & \ldots & \\ \ldots & & & & \\ 0 & \ldots & 1 & c_i & a_i \end{pmatrix}$$

and follows directly from (A1) and from the Kramer rule.

References

Bassichis W H and Strayer M R 1978 *Phys. Rev.* C **18** 1505
Graffi S and Grecchi V 1975 *Lett. Nuovo Cimento* **12** 425
Grund F 1977 *Zh. Vychisl. Mat. Fiz.* **17** 1117–22
Haydock R and Kelly M J 1975 *J. Phys. C: Solid State Phys.* **8** L290–3
Killingbeck J 1977 *Rep. Prog. Phys.* **40** 963–1031
Korn G A and Korn T M 1968 *Mathematical Handbook* (New York: McGraw-Hill)
Richardson J L and Blankenbecler R 1979 *Phys. Rev.* D **19** 496
Wall H S 1948 *Analytic Theory of Continued Fractions* (New York: Van Nostrand)
Znojil M 1976 *J. Phys. A: Math. Gen.* **9** 1–10
—— 1977 *J. Math. Phys.* **18** 717
—— 1978 *J. Phys. A: Math. Gen.* **11** 1501–8
—— 1981 *Lett. Math. Phys.* **5** 405–9
—— 1983 *J. Phys. A: Math. Gen.* **16** 213–20