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Schrödinger equation as recurrences: III. Partitioning approach

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Abstract. In the generalised Lanczos basis, we partition the Hamiltonian to tridiagonal form and, *mutatis mutandis*, apply the ideas of I and II. It solves the Schrödinger eigenvalue problem again. The resulting method modifies and complements our formalism and simplifies its use and interpretation. As an example of application, the unique asymptotical effective Hamiltonian is derived. Also, for the anharmonic oscillators, the convergence of its continued fractional definition is proved and the compact formula for the higher-order asymptotic corrections is found.

1. Introduction

In this paper we intend to combine the preceding backward-running (I, Znojil 1983b) and forward-running (II, Znojil 1984) recurrent treatments of the Schrödinger equation

$$H\psi = E\psi \tag{1.1}$$

into a unified picture. Let us start this development by repeating the main assumptions.

First, we assume that (1.1) is represented in the generalised Lanczos basis $|n\rangle$, $n = 1, 2, \ldots$. Then, the matrix

$$\langle m|H|n\rangle = \mathscr{H}_{mn} + E\delta_{mn} \tag{1.2}$$

is non-zero if and only if $|m-n| \leq t$.

The positive integer t defines the partitioning

$$\mathscr{H} = \begin{pmatrix} A_1 & B_1 & & \\ C_2 & A_2 & B_2 & \\ & C_3 & A_3 & B_3 \\ & & \cdots & \end{pmatrix}, \qquad \dim A_{k+1} = t, \qquad k \geq 1 \tag{1.3}$$

as introduced in I, while $M = \dim A_1 > 0$ is an independent variable needed for formal reasons only.

Next, we assume that the asymptotic form of the Hamiltonian is simple enough,

$$\mathscr{H}_{M+1+mM+1+n} \approx \frac{1}{\tau_{M+1+m}} \tau_{M+m}\mathscr{H}_{M+mM+n}\sigma_{M+n} \cdot \frac{1}{\sigma_{M+1+n}}, \qquad M \gg 1 \tag{1.4}$$

i.e., that it exhibits constant-matrix behaviour after re-scaling in the asymptotic region.

Finally, we have to assume that the Hamiltonian can be factorised as in I:

$$\tau\mathscr{H}\sigma=\gamma\prod_{i=1}^{t}U^{(i)}\prod_{j=1}^{t}U^{(i+j)\mathrm{T}} \tag{1.5}$$

$$U^{(k)}=\begin{pmatrix}1 & \alpha_1^{(k)} & 0 & \dots \\ 0 & 1 & \alpha_2^{(k)} & 0\dots \\ 0 & 0 & 1 & \alpha_3^{(k)}\dots \\ & \dots & & \end{pmatrix}$$

and also satisfies the asymptotic smoothness requirement in a 'strong' form:

$$\lim_{k\to\infty}\alpha_k^{(i)}=\alpha^{(i)}. \tag{1.6}$$

Now, we may summarise briefly the contents of I as a definition of the parameters $\alpha^{(i)}\in(-1,1)$ (as functions of the matrix elements of $\mathscr{H}$ in the asymptotic region), while II uses these parameters as input into the definition of the physical boundary conditions for recurrences. In I and II, we have also obtained two non-equivalent finite-dimensional equivalents of the whole infinite-dimensional Schrödinger equation in an appropriate leading-order (and systematically improvable) approximation.

From the methodical point of view, I and II have interpreted the recurrences (1.1), i.e.

$$\prod_{n=\max(1,m-t)}^{m+t}\mathscr{H}_{mn}z_n=0,\qquad z_n=\langle n|\psi\rangle,\qquad m=1,2,\dots \tag{1.7}$$

as initialised at $m=\infty$ and $m=1, 2, \dots, t$, respectively. In the present continuation, the remaining possibility of initialising (1.7) at some intermediate values of m will be added to the formalism, and its partitioned re-formulation will be given.

In § 2, we introduce three auxiliary projectors as in Feshbach (1958), corresponding, respectively, to the domain of initialisation and both directions of recurrences in the general case.

In § 3, we concentrate on the forward-running recurrences and re-express the compact definition II of the regular general solution in the partitioned notation. We may shift the indices and, in particular, use the generalised (shifted) initialisations. Of course, the physical boundary conditions remain the same as in II.

In § 4, we re-investigate the backward-running matrix continued fractional (MCF) recurrences of I. In the purely algebraic setting, their initialisation is shown to be (almost) arbitrary. The second partitioned representation of the regular solution is also obtained.

In § 5, we consider the 'exactly solvable' anharmonic oscillator (AHO) example in the asymptotic region, as an illustration of the present forward–backward-symmetric recurrent approach. We show that the ambiguities of G_k (§ 4) are only 'local' and compensated, in effect, by the convergence properties.

In § 6, the exceptional AHO properties inspire us to reparametrise (and to simplify significantly) the physical asymptotics (and the general formulae of I). In this way, the partitioned generalisation of II is completed.

Numerical applications are omitted in the present methodical series. Nevertheless, the whole class of the AHO examples permits us to construct the higher-order perturbation corrections still by the purely algebraic means. Such a procedure appears to be surprisingly straightforward and is described in detail in the appendix.

2. Triple partitioning

In accordance with theorem 1 of II, each t-plet of projections

$$\langle n_i|\psi\rangle = z_{n_i}, \qquad n_i < \infty, \qquad i=1,2,\ldots,t \tag{2.1}$$

is defined by the 'initial' parameters $z_1, z_2, \ldots, z_t$ and by the recurrences (1.7) and *vice versa*, we may start directly from the shifted initialisation (2.1) and try to define the general solution z_k, $k \geq 1$, in full analogy with the determinantal formula (2.2) of II.

To simplify the notation, we may assume that all the values (2.1) lie within a 'model space' specified by the projector P. Provided that the dimension of this space is large enough, we may decompose the unit projector in such a way that

$$R+P+Q=1, \qquad Q\mathscr{H}R = R\mathscr{H}Q = 0. \tag{2.2}$$

This reflects the band-matrix character of $\mathscr{H}$.

As a consequence, the triply partitioned Schrödinger equation (1.7)

$$\begin{aligned} &R\mathscr{H}Rz + R\mathscr{H}Pz = 0\\ &P\mathscr{H}Rz + P\mathscr{H}Pz + P\mathscr{H}Qz = 0\\ &Q\mathscr{H}Pz + Q\mathscr{H}Qz = 0 \end{aligned} \tag{2.3}$$

permits us to eliminate Qz and Rz in a purely formal way,

$$\begin{aligned} &\mathscr{H}^{\text{eff}}Pz = 0\\ &\mathscr{H}^{\text{eff}} = P\mathscr{H}P - P\mathscr{H}Q(Q\mathscr{H}Q)^{-1}Q\mathscr{H}P - P\mathscr{H}R(R\mathscr{H}R)^{-1}R\mathscr{H}P. \end{aligned} \tag{2.4}$$

Provided that the symbols $(Q\mathscr{H}Q)^{-1}$ and $(R\mathscr{H}R)^{-1}$ are interpreted as limits of the finite-dimensional matrix inverses (using, e.g., a variational interpretation of (2.3)), the Feshbach-type, finite-dimensional equation (2.4) is exact and equivalent to equation (2.3).

In the non-symmetric cases of the type (1.3), the variational background of (2.3) may become questionable sometimes (cf, e.g., Schwartz 1965). Then, a rigorous alternative formulation of the formal and solvable equivalents to (2.3) may be done still using the methods of II.

Starting from the detailed block structure (1.3) of $\mathscr{H}$, we may write the projectors in a 'canonical' form

$$\begin{aligned} &R = \sum_{m=1}^{M-2t+m_1 t} |m\rangle\langle m|, && m_1 \geq 1\\ &P = \sum_{m=M-2t+m_1 t+1}^{M-t+m_2 t} |m\rangle\langle m|, && m_2 \geq m_1\\ &Q = \sum_{m=M-t+m_2 t+1}^{\infty} |m\rangle\langle m| \end{aligned} \tag{2.5}$$

with the variable dimension of A_1 again. For the sake of definiteness, we may also assume that $m_2 > m_1$ and obtain the fully general effective Hamiltonian (2.4) in the partitioned form

$$\mathscr{H}^{\text{eff}} = \begin{pmatrix} F_{m_1} & B_{m_1} & & \\ C_{m_1+1} & A_{m_1+1} & B_{m_1+1} & \\ & \cdots & & \\ & C_{m_2} & G_{m_2} & \end{pmatrix}, \qquad m_2 > m_1. \tag{2.6}$$

Obviously, it differs from the $P\mathscr{H}P$ projection of the original band-matrix Hamiltonian in the modified blocks (submatrices) A_{m_1} and A_{m_2} only. In an implicit way, they are defined by (2.4) in the variational cases.

3. Shifted initialisations and the partitioned regular type solutions

In a non-variational interpretation of the Schrödinger equation (1.7) or (2.3), we have to re-consider the definition of $\mathscr{H}^{\text{eff}}$. We shall see that (2.4) need not fix the energies and *vice versa*, its modified or usual truncation definition may also be derived in a non-variational manner.

Of course, the finite-dimensional R-projected 'upper' subspace cannot cause any trouble at all—the first auxiliary sequence of the effective Hamiltonian submatrices F_k is uniquely defined by the simple inversion

$$F_1 = A_1, \qquad F_k = A_k - C_k(F_{k-1})^{-1}B_{k-1}, \qquad k = 2, 3, \ldots. \tag{3.1}$$

Here, any random singularities are to be removed by an appropriate change of M. Then, the recurrences

$$\begin{pmatrix} z_{n+1} \\ z_{n+2} \\ \cdots \\ z_{n+r} \end{pmatrix} = X_m = -(F_m)^{-1}B_m X_{m+1} \tag{3.2}$$

(with $n = M + (m-2)t$ and $r = t$ for $m \geqslant 2$, or $n = 0$ and $r = M$ for $m = 1$) also become well defined and enable us to re-construct easily the R-projected part of the z-solution from our knowledge of Pz.

Concerning the Q-projected part of the infinite-dimensional vector z, it may be generated by the reversed formula

$$X_{m+1} = -(B_m)^{-1}F_m X_m = (-1)^{m-1}\left(\prod_{k=0}^{m-2} B_{m-k}^{-1}F_{m-k}\right)X_2. \tag{3.3}$$

It represents a partitioned analogue of the (recurrently defined) determinantal solution as given in II. Alternatively, we may use (3.3) only to define some Q-projected and 'compactified' shifted initialisations

$$z_{n+i}, \qquad i = 1, 2, \ldots, t, \qquad n = M + t\times(m-2). \tag{3.4}$$

Then, after an appropriate shift of indices, we may also use the closed determinantal definition ((2.2) of II) of the general (non-truncated) regular-type solution again.

A discussion of the corresponding physical asymptotic boundary conditions remains of course the same as in § 3 of II. We may re-emphasise that they are precisely equivalent to the normalisability requirement and entirely independent of the particular truncative or variational additional assumptions.

4. Re-interpretation of the effective Hamiltonians

Recurrences (3.1) may be generated by a simple factorisation prescription

$$\mathcal{H}=\begin{pmatrix} A_1 & B_1 & \\ C_2 & A_2 & B_2 \\ & \dots & \end{pmatrix}=\begin{pmatrix} I & & \\ C_2/F_1 & I & \\ & C_3/F_2 & I \\ & \dots & \end{pmatrix}\times\begin{pmatrix} F_1 & B_1 & & \\ & F_2 & B_2 & \\ & & F_3 & \\ & & \dots & \dots \end{pmatrix} \tag{4.1}$$

$$F_1=A_1,\qquad F_k=A_k-C_k(F_{k-1})^{-1}B_{k-1},\qquad k=2,3,\dots.$$

Its formal counterpart may be related also to the recurrences introduced in I

$$\mathcal{H}=\begin{pmatrix} I & B_1/G_2 & \\ & I & B_2/G_3 \\ & & \dots \end{pmatrix}\times\begin{pmatrix} G_1 & & \\ C_2 & G_2 & \\ & C_3 & G_3 \\ & & \dots \end{pmatrix} \tag{4.2}$$

$$G_k=A_k-B_k(G_{k+1})^{-1}C_{k+1},\qquad k=1,2,\dots.$$

In the light of the preceding paragraph, this may be understood also as a transition to the 'lower', Q-projected space. Now, contrary to the preceding case, any initialisation may be used due to the infinite dimension of Q.

To clarify the latter point, let us put formally

$$\begin{pmatrix} G_1 & & \\ C_2 & G_2 & \\ & C_3 & G_3 \\ & & \dots \end{pmatrix}\begin{pmatrix} X_1 \\ X_2 \\ X_3 \\ \dots \end{pmatrix}=\begin{pmatrix} W_1 \\ W_2 \\ W_3 \\ \dots \end{pmatrix}. \tag{4.3}$$

This is precisely equivalent to the Schrödinger recurrences (1.7) if and only if we satisfy the relations

$$W_k+B_k(G_{k+1})^{-1}W_{k+1}=0,\qquad k=1,2,\dots. \tag{4.4}$$

Now, with respect to the structure of the generalised Lanczos basis as mentioned in II, there exists k_0 such that $\det B_k\neq 0$ for all $k\geqslant k_0$—we may define all the vectors W_k from the initialisation W_{k_0} by means of (4.4). It is necessary to emphasise that all these initialisations are equivalent from the present point of view—their change only modifies definition (4.3) of the solution in terms of the auxiliary matrices G_k. Hence, in full analogy with the $t=1$ example (Znojil 1983a), it is reasonable to pick up W_{k_0} $(=W_k,\ k=1,2,\dots)=0$ in what follows. It has the following three merits.

(1) Since $G_1=G_1(W_1)$ in general, we suppress the purely formal ambiguity of the physical effective Hamiltonian and make it compatible with its particular (truncation) standard interpretation.

(2) It simplifies (4.3) and the asymptotic-behaviour analysis of z,

$$\begin{aligned} X_{m+1}&=-(G_{m+1})^{-1}C_{m+1}X_m=\left(\prod_{i=0}^{m-1}-\frac{1}{G_{m+1-i}}C_{m+1-i}\right)X_1,\\ m&=1,2,\dots,\qquad G_1X_1=0. \end{aligned} \tag{4.5}$$

(3) It still permits us to vary the boundary conditions for G_k, which is equivalent also to theorem 1 of II.

Theorem 1. Irrespective of their initialisation, recurrences (4.2) may be used to generate the general solution z of the infinite linear set (1.7) by the partitioned prescriptions

$$X_n = -(C_{n+1})^{-1} G_{n+1} X_{n+1}, \qquad n \geq 2 \tag{4.6}$$

and (4.5), provided only that the t-dimensional equation

$$\mathscr{H}^{\mathrm{eff}(m)} X_m = 0, \qquad \mathscr{H}^{\mathrm{eff}(m)} = A_m - F_m - G_m \tag{4.7}$$

is satisfied at some $m \geq 1$.

Proof. In analogy with (2.6), the 'most economical' effective $t \times t$ Hamiltonian may be defined in the 'minimal' model space with $m_1 = m_2$—equation (4.7) merely re-expresses the zero choice of the quantities W_i in (4.3). Then, the insertion (of z resulting from (4.5) and (4.6)) leads to the direct verification of the Schrödinger recurrences (2.3).

The physical normalisability requirements should be imposed on X_n in the same way as in II. Presumably, they may be related also to $\mathscr{H}^{\mathrm{eff}(m)}$, $m \gg 1$, at least in the MCF solvable cases. Then, the variations of $G_N \neq A_N$ may become a basis for a systematic acceleration of convergence of the related algorithms.

5. The effective Hamiltonians in the asymptotic region and their AHO example

From the assumption (1.4), the asymptotic part of the Hamiltonian $\mathscr{H}$ may be written in the form

$$\mathscr{H} \sim \begin{pmatrix} \cdots & & & & \\ & c & a & b & \\ & & c & a & b \\ & & & & \cdots \end{pmatrix}. \tag{5.1}$$

Thus, up to the same diagonal scaling factors τ and σ, we may also consider the partitioned and asymptotic form of the effective Hamiltonian (4.3) with $m_2 > m_1 \gg 1$ and denote

$$\mathscr{H}^{\mathrm{eff}} \sim \begin{pmatrix} f & b & & & \\ c & a & b & & \\ & & \cdots & & \\ & & c & a & b \\ & & & c & g \end{pmatrix}. \tag{5.2}$$

Here, the only unknown 'effective' submatrices $f = f_\infty$ and $g = g_\infty$ may be defined by the simple MCF-type iterative formulae

$$\begin{aligned} g_{k+1} &= a - b(g_k^{-1})c \\ f_{k+1} &= a - c(f_k)^{-1} b \end{aligned} \tag{5.3}$$

with an appropriate initialisation.

In the particular AHO example with

$$a_{ij} = \binom{2t}{t+i-j}, \qquad b_{ij} = c_{ji} = \binom{2t}{i-j}, \qquad i, j = 1, 2, \ldots, t \tag{5.4}$$

(cf both I and II), the matrices f_∞ and g_∞ may be computed simply from the exactly solvable quadratic equations

$$g_\infty = a + b(g_\infty^{-1})c, \qquad f_\infty = a - c(f_\infty)^{-1}b \tag{5.5}$$

for the $t\times t$-dimensional matrices.

Lemma 1. Provided that (5.1) coincides with the AHO example

$$\begin{aligned} &\mathcal{H}_{M+mM+n} = c_1 M^{c_2} h_{mn}(t)(1+O(1/M)) \\ &h_{mn}(t) = \binom{2t}{t+m-n}, \qquad m, n-1, 2, \ldots \end{aligned} \tag{5.6}$$

in the asymptotic region, we have the unique leading-order formulae

$$\begin{aligned} &F_{m_1} \doteq c_1 M^{c_2} S^{\mathrm{T}} S, \qquad S_{ij} = S_{ij}(t) = \binom{t}{j-i}, \qquad i, j = 1, 2 \ldots t \\ &G_{m_2} \doteq c_1 M^{c_2} S S^{\mathrm{T}}, \qquad m_1, m_2 \geqslant 2, \qquad M = M_1 \gg 1 \end{aligned} \tag{5.7}$$

defining the effective Hamiltonian (4.7) in an explicit way.

Proof. This lies in mere re-formulation of § 3.2 of I. The uniqueness of (5.7) follows from the t-times degenerate character of the factorisation as defined by theorem 2 in I.

In the iterative prescriptions (5.3), the unique fixed points (5.7) are merely semi-stable. Fortunately, whenever the iterations start from a larger matrix $g_k > g_\infty$ or $f_k > f_\infty$, they remain stable—this generalises the $t = 1$ result of Znojil (1983a).

Lemma 2. In the AHO example (5.4), the MCF form of

$$g_\infty = a - b\cfrac{1}{a - b\cfrac{1}{a - \ldots}c}c \tag{5.8}$$

converges to the value SS^{T} for any integer $t \geqslant 1$. The difference $g_k - g_\infty$ is positive definite for the finite MCF approximants g_k.

Proof. Let us denote

$$\begin{aligned} &g_k = SS^{\mathrm{T}} + S^{\mathrm{T}}\delta_k S, \qquad \delta_1 = 1 \\ &\delta_{k+1} = 1 - \frac{1}{1 + S^{-1}S^{\mathrm{T}}\delta_k S S^{\mathrm{T}-1}} = \frac{1}{1 + \gamma^{\mathrm{T}}(1/\delta_k)\gamma}, \qquad \gamma = \frac{1}{S^{\mathrm{T}}} S. \end{aligned} \tag{5.9}$$

Then, the Mth MCF iterate is simple since $b = S^{\mathrm{T}}S^{\mathrm{T}}$, $a = SS^{\mathrm{T}} + S^{\mathrm{T}}S$ and

$$\frac{1}{\delta_M} = 1 + \sum_{k=1}^{M} (\gamma^{\mathrm{T}})^k \gamma^k. \tag{5.10}$$

It is a positive definite matrix with the real eigenvalues $\lambda_i^{(M)} > 1$. This follows from the minimax property of a sum of matrices (Wilkinson 1965) and implies that all the

Table 1. Anharmonic oscillator example—the eigenvalues of $1/\delta_M$ for $t=2$.

M	$\lambda_1^{(M)}$	$\lambda_2^{(M)}$
0	1.0000	1.0000
1	18.9442	1.0557
2	84.7612	1.2387
3	230.5425	1.4574
4	488.3105	1.6894
5	890.0720	1.9279
6	1467.8301	2.1698
7	2253.5860	2.4149
8	3279.3406	2.6593

eigenvalues $\mu_i^{(M)} = 1/\lambda_i^{(M)}$ of δ_M lie within the interval (0, 1). They decrease monotonically with increasing M (see table 1 as an example). Indeed, the matrix difference

$$(\gamma^{\mathrm{T}})^{M+1}\gamma^{M+1} = \frac{1}{\delta_{M+1}} - \frac{1}{\delta_M} \tag{5.11}$$

has positive eigenvalues only (see Wilkinson 1965). This process may stop at the fixed point δ_∞ only, and this point is unique and equal to zero.

We may summarise: for a class of initialisations (including the MCF one), the sequence G_k (similarly F_k) has a unique point of accumulation. The asymptotic AHO effective $m_1 = m_2$ Hamiltonian becomes identically equal to zero: in the given approximation, (4.7) does not restrict the t-parametric freedom in the asymptotic initialisations at all. In order to remove this degeneracy of the physical and non-physical asymptotic boundary conditions, we must take the higher-order corrections into account.

A priori, the corrections may have a non-matrix, one-parametric character. Such behaviour is confirmed numerically in table 1 for the $t=2$ AHO system. In this example, an ordering of corrections and separation of the quickly and slowly convergent MCF components may also be achieved by non-numerical means.

Lemma 3. In the $t=2$ AHO example, we encounter the one-parametric behaviour of the second-order MCF corrections

$$g_k = \begin{pmatrix} 5 & 2 \\ 1 & 1 \end{pmatrix} + \lambda_k \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + \mathrm{O}(\lambda_k^2), \qquad 1 \gg \lambda_k > \lambda_{k+1} \geqslant 0 \tag{5.12}$$

in the $k \gg 1$ asymptotic region.

Proof. Since

$$S = \begin{pmatrix} 1 & 2 \\ 0 & 1 \end{pmatrix}, \qquad \gamma = \begin{pmatrix} 1 & 2 \\ -2 & -3 \end{pmatrix}, \qquad a = \begin{pmatrix} 6 & 4 \\ 4 & 6 \end{pmatrix}, \qquad b = \begin{pmatrix} 1 & 0 \\ 4 & 1 \end{pmatrix}$$

we have

$$\gamma^k = (-1)^k \begin{pmatrix} -(2k-1), & -2k \\ 2k, & 2k+1 \end{pmatrix},$$

$$\frac{1}{\delta_N} = 1 + \sum_{k=1}^{N} \gamma^{\mathrm{T}k}\gamma^k = \begin{pmatrix} 1+\psi(2N), & 8\psi(N) \\ 8\psi(N), & \psi(2N+1) \end{pmatrix}$$

$$\psi(k) = \tfrac{1}{6}(2k^3 + 3k^2 + k). \tag{5.13}$$

Hence, the inversion of $[\delta_N^{-1}]_{mn}$ is ill conditioned for $N \gg 1$,

$$\frac{1}{\delta_N} = 8N^3\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + O(N^2).$$

The exact computation recovers that the cancellations take place in the first two asymptotic orders,

$$\det \frac{1}{\delta_N} = \tfrac{1}{12}(N^4 + 8N^3 + 23N^2 + 28N + 12) = \tfrac{1}{12}(N+1)(N+2)^2(N+3).$$

Hence, we have $\delta_N = O(1/N)$ as required by the smallness of the corrections, and formula (5.12) follows.

When we insert (5.12) into (5.3), an iterative formula for λ_k will be obtained. In this formula, the higher-order corrections may be added as well, for example for us to estimate the errors. For further details and the generalisation of lemma 3, see the appendix.

6. The partitioned boundary conditions

6.1. *The natural parametrisation of $Q\mathcal{H}Q$*

Let us introduce the parametrisation

$$\mathcal{H}_{M+mM+n} = \text{constant}(M)[h(t) + \rho_1 h(t-1) + \cdots + \rho_{t-1} h(1) + \rho_t]_{mn}(1 + O(1/M))$$

$$h_{mn}(t) = \binom{2t}{t+m-n} \tag{6.1}$$

of the symmetric and smooth matrix $\mathcal{H}$. It is inspired by the above AHO example and reflects its exceptional character: t-tuple degeneracy, slow convergence and non-applicability of the geometric convergence criterion of theorem 3 of I, etc. Moreover, it also simplifies the general results of I:

Theorem 2. In the algebraic factorisation (1.5) of (6.1)

$$h(t) + \sum_{i=1}^{t} \rho_i h(t-i) = \left[\prod_{i=1}^{t} \alpha_i^{-1} I_{(+)}(\alpha_i)\right] \times \prod_{j=1}^{t} I_{(+)}^{T}(\alpha_j)$$

$$[I_{(+)}(\alpha)]_{mn} = \delta_{mn} + \alpha\delta_{m+1n}, \qquad m, n = 1, 2, \ldots \tag{6.2}$$

in terms of the matrices $U \equiv I_{(\pm)}$, the parameters

$$\alpha_i = \alpha_i^{(\pm)} = e^{\pm\beta_i}, \qquad 4sh^2\beta_i/2 = Y_i, \qquad i = 1, 2, \ldots t \tag{6.3}$$

exhibit the $\alpha_i \leftrightarrow 1/\alpha_i$ ambiguity and are given by the roots of the algebraic equation

$$Y^t - \rho_1 Y^{t-1} + \rho_2 Y^{t-2} - \ldots + (-1)^t \rho_t = 0. \tag{6.4}$$

Proof. This is merely a re-arrangement of the proof given in I for theorem 2. Indeed, the change of variables gives precisely equation (16) of I.

6.2. *The physical wavefunctions*

When we define Qz by means of the factorised inversion of $Q\mathscr{H}Q$, $Qz = -(Q\mathscr{H}Q)^{-1}Q\mathscr{H}Pz$, we put, in accordance with I or (6.2),

$$Qz \doteq \left[\prod_{j=1}^{t} I_{(+)}^{\mathrm{T}^{-1}}(\alpha_j)\right] \times \prod_{i=1}^{t} \alpha_i I_{(+)}^{[t]^{-1}}(\alpha_i) \times \begin{pmatrix} c_1 \\ c_2 \\ \dots \\ c_t \end{pmatrix}. \tag{6.5}$$

Then, the normalisable solutions of (1.7) have a simple structure and they may be classified easily.

Theorem 3. Provided that $\rho_i > 0$, $i = 1, 2, \dots, t$ and

$$\begin{aligned}
&t = 2, \qquad \rho_1^2 > 4\rho_2, \text{ or} \\
&t = 3, \qquad 4(\rho_1^2 - 3\rho_2)^3 > (q\rho_1\rho_2 - 2\rho_1^3 - 27\rho_3)^2, \text{ or} \\
&t = 4, \qquad 3\rho_1^2 > 8\rho_2, \\
&\qquad \tfrac{1}{16}(3\rho_1^2 - 8\rho_2)^2 > 12\rho_4 + \rho_2^2 - 3\rho_1\rho_3 \\
&\qquad\qquad > 4^{-1/3}|27\rho_3^2 - 72\rho_2\rho_4 + 2\rho_2^3 - 9\rho_1\rho_2\rho_3 + 27\rho_1^2\rho_4|^{2/3},
\end{aligned} \tag{6.6}$$

etc, the parameters $\alpha_i \neq 1$ will be real. Then, the solutions of (1.7) as given by (24) in I, i.e.,

$$\begin{pmatrix} z_{M+1} \\ z_{M+2} \\ \dots \end{pmatrix} = \sum_{i=1}^{t} \nu_i \times \begin{pmatrix} -\alpha_i \\ +\alpha_i^2 \\ -\alpha_i^3 \\ \dots \end{pmatrix}, \qquad M \gg 1 \tag{6.7}$$

will be normalisable if and only if we put $\alpha_i = \alpha_i^{(-)}$ for all $i = 1, 2, \dots, t$ in (6.7).

Proof. This starts from the simplicity of (6.4) and it complements only theorem 3 of I by the conditions guaranteeing the positivity of the roots, i.e., $0 < \alpha_i^{(-)} < 1 < \alpha_i^{(+)} < \infty$.

6.3. *The physical asymptotics of* $\mathscr{H}^{\text{eff}}$

The preceding results enable us to interpret and remove simply the ambiguity as mentioned in theorem 2.

Theorem 4. From the asymptotically smooth Hamiltonian (5.1) factorised by means of the formulae (6.1) and (6.2), the unique asymptotical effective Hamiltonian (5.2) with $M \gg 1$ may be defined by the products

$$g = \left[\prod_{i=1}^{t} \alpha_i^{-1} I_{(+)}^{[t]}(\alpha_i)\right] \times \prod_{j=1}^{t} I_{(+)}^{[t]\mathrm{T}}(\alpha_j) \tag{6.8}$$

and

$$f = \left[\prod_{i=1}^{t} \alpha_i^{-1} I_{(+)}^{[t]\mathrm{T}}(\alpha_i)\right] \times \prod_{j=1}^{t} I_{(+)}^{[t]}(\alpha_j)$$

$$[I_{(+)}^{[t]}(\alpha)]_{mn} = \delta_{mn} + \alpha\delta_{m+1\,n}, \qquad m, n = 1, 2, \dots, t \tag{6.9}$$

of the $t\times t$-dimensional submatrices $I_{(+)}^{[t]}$ of $I_{(+)}$. The physical requirements fix $\alpha_i=\alpha_i^{(-)}$ and $\alpha_i=\alpha_i^{(+)}$ in (6.8) and (6.9), respectively.

Proof. This follows from formula (10) in I and merely represents the fixed-point solution of the quadratic equations (5.5) combined with the relations (6.5), (3.3) and with theorem 3. In the light of the identity

$$(JKJ)_{mn}=K_{t-m+1\,t-n+1},\qquad J=\begin{pmatrix}0\dots0 & 1\\ 0\dots1 & 0\\ \dots & \\ 1 & 0\dots0\end{pmatrix}\tag{6.10}$$

both the formulae are equivalent since $JI_{[+]}^{[t]}J=I_{(+)}^{[t]\mathrm{T}}$.

For the slowly convergent AHO-type cases with $\rho_i\ll 1$ in (6.1) and $1-\max|\alpha_i|$ close to zero, we have arrived at a complete generalisation of our recent $t=1$ discussion (Znojil 1983a). Thus, the initialisations (or boundary conditions) (6.7) and (5.2) may be used in the recurrent prescriptions (3.2)–(3.3) or (4.5)–(4.6) as a basis of accelerated algorithms of the MCF type, as well as of the various asymptotic expansions and approximate formulae.

7. Outlook and summary

In this series of papers, an emphasis has been laid upon the recurrent algebraic structure of the Schrödinger-type band-matrix equation (2.1). Its physical solutions are specified symmetrically by the initial and asymptotic boundary conditions in a way paralleling the theory of ordinary differential equations.

In this paper, we have modified the standard introduction of the auxiliary effective-Hamiltonian submatrices. The physical normalisability requirement then acquires a new understanding: among a finite number of the MCF fixed-points, it chooses the unique physical effective interaction given by the compact formula.

In the forthcoming computations, various eigenvalue algorithms may be based on an analysis of stability of the matrix quadratic-equation roots (with respect to the underlying iterations). Besides a re-derivation and important improvements of the variational MCF-type techniques, some new non-variational (e.g., Hill-type) approaches may also be derived from the formalism. Their description and tests have been deferred to a subsequent publication.

Appendix. Convergence of the auxiliary matrix continued fractions and its acceleration

Being inspired by the degenerate character of the AHO example in § 5, let us consider now the parameters ρ_i in § 6 as small corrections. Obviously, with the variational (MCF and trivial) $g_1=f_1=a$ initialisation of the auxiliary matrix sequences (5.3), only small deviations from the AHO results (lemmas 1–3) may be expected. Hence, the MCF convergence of g_∞ (and, similarly, of f_∞ of course) may be efficiently accelerated by subtractions

$$g_k = g_k^{(\mathrm{AHO})} + g_k^{(\mathrm{new})} \tag{A1}$$

in full analogy with the classical analytic continued fraction theory (Wall 1948). Now, we shall therefore describe the structure and k-dependence of the 'known' MCF quantities $g_k^{(\mathrm{AHO})}$ in more detail. Our study will be based on equation (5.9) and on an expansion of the matrices γ and δ_k in an appropriate bra and ket basis.

Dimension $t=2$

The direct way to solve our problem is to compute the explicit formulae for δ_k—this was done in the proof of lemma 3. In principle, this procedure may be used for $t>2$ as well, but the related algebra becomes very clumsy. Hence, we shall now describe the $t=2$ method permitting an easy generalisation. It is based on the combinatorial identities in the corresponding formulae, and on an intuitive, though systematic, guess of the optimal parametrisations. So, with $t=2$ we put

$$\gamma = \begin{pmatrix} 1 & 2 \\ -2 & -3 \end{pmatrix} = -I + 2|u\rangle\langle v|, \qquad \langle v| = (1,1), \qquad \langle u| = (1,-1).$$

This formula has the simple properties

$$\langle u|u\rangle = \langle v|v|\rangle = 2, \qquad \langle u|v\rangle = \langle v|u\rangle = 0$$

which imply immediately that

$$\gamma^k = (-1)^k(I - 2k|u\rangle\langle v|)$$
$$\gamma^{kT}\gamma^k = I - 2k(|v\rangle\langle u| + |u\rangle\langle v|) + 8k^2|v\rangle\langle v|.$$

Thus, we may write

$$1/\delta_N = z_1 + z_2(|v\rangle\langle u| + |u\rangle\langle v|) + z_3|v\rangle\langle v|$$

$$z_1 = N+1, \qquad z_2 = -2\sum_{k=1}^{N} k = -N(N+1), \qquad z_3 = 8\sum_{k=1}^{N} k^2 = \tfrac{4}{3}N(N+1)(2N+1)$$

which reproduces (5.13) in a more elegant form. The final inverse then follows from the identity $2 = |u\rangle\langle u| + |v\rangle\langle v|$ and reads

$$\delta_N = y_1|u\rangle\langle u| + y_2(|u\rangle\langle v| + |v\rangle\langle u|) + y_3|v\rangle\langle v|$$
$$y_1 = (z+1/2)/\Delta, \qquad y_2 = N/\Delta, \qquad y_3 = 1/2\Delta \tag{A2}$$
$$\Delta = (N+1)(2z - 4N^2 + 1), \qquad z = \tfrac{4}{3}N(2N+1).$$

In the second-order approximation, we obtain (5.12) again.

Dimension $t \geqslant 2$

The main feature of (A2) is the separation of corrections with respect to their orders of magnitude. Hence, the one-parametric, essentially non-matrix (and, hence, non-numerical) character of the estimate (5.12) appears to be preserved in the higher-order corrections as well. The same phenomenon may be observed at the higher dimensions t and stems from the same reason, namely, from the projector-type character of the matrices $\gamma \pm 1$.

After a short computation, we may determine the sign in these matrices, find that $\det(\gamma(t)+(-1)^t)=0$ and put

$$\gamma=\gamma(t)=(-1)^{t+1}I+\sum_{i=1}^{t-1}|u_i\rangle M_{ii}^{(1)}\langle v_i|. \tag{A3}$$

The trial choice of

$$\begin{aligned}\langle v_1| &= (0,0,\ldots 0,1,1)\\ &\ldots\\ \langle v_k| &= \left(\binom{k}{k-t+1},\binom{k}{k-t+2},\ldots,\binom{k}{k-1},\binom{k}{k}\right)\\ \langle v_{t-1}| &= \left(1,t-1,\binom{t-1}{2},\ldots,t-1,1\right)\end{aligned} \tag{A4}$$

leads to the possibility of picking up $\langle u_1|=(1,\,-1,\,1,\,-1,\,\ldots,\,(-1)^{t+1})$ such that

$$(-1)^{t+1}|u_1\rangle=\gamma(t)|u_1\rangle, \qquad \langle v_i|u_1\rangle=0, \qquad i=1,2,\ldots,t-1. \tag{A5}$$

The form of the remaining $|u_i\rangle$ vectors follows from (A3) and its sample is given in table 2 for a few values of t. In general, their generation is easily done by the recurrent symbolic manipulations on the computer.

Table 2. Overlaps in the non-orthogonal basis.

t	i	$\langle u_i|$	$M_{ii}^{(1)}$	(j,k)	$G_{jk}\neq 0$
2	1	(1, −1)	2	—	
3	1	(1, −1, 1)	3	(1, 2)	1
	2	(0, −1, 2)	3		
4	1	(1, −1, 1, −1)	2	(1, 3)	−6
	2	(1, 3, 5, 7)	2	(1, 2)	−4
	3	(0, 1, 4, 9)	2	(2, 3)	−2
5	1	(1, −1, 1, −1, 1)	5	(1, 4)	7
	2	(−1, 0, 1, −2, 3)	5	(1, 3), (2, 4)	3
	3	(1, −1, 2, −4, 7)	5	(1, 2), (2.3), (3, 4)	1
	4	(0, −1, 3, −7, 14)	5		

In the next step, we may write

$$\gamma^m(t)=(-1)^{(t+1)m}I+\sum_{i,j=1}^{t-1}|u_i\rangle M_{ij}^{(m)}\langle v_j| \tag{A6}$$

which leads to the recurrences

$$M^{(m+1)}=(-1)^{t+1}M^{(m)}+(-1)^{(t+1)m}M^{(1)}+M^{(1)}GM^{(m)}. \tag{A7}$$

Here, the most important property of the overlap matrix $G_{ij}=\langle v_i|u_j\rangle$ is its nilpotent character, $G^{t-1}=0$. This may be derived most easily from the nilpotence of the matrix $S-1$ (see (5.7)) and implies our main result:

Theorem 5. After N iterations of the AHO MCF mapping $g_1 \to g_2 \to \ldots \to g_{N+1}$, we get the estimate of the type (5.12)

$$g_{N+1} = SS^{\mathrm{T}} + \frac{\lambda^{(1)}(N)}{N} |v_{t-1}\rangle\langle v_{t-1}| \sum_{i=2}^{2t-1} \sum_{k=1}^{i} \frac{\lambda_k^{(i)}(N)}{N^i} S^{\mathrm{T}} |v_{k-1}\rangle\langle v_{i-k}| S \tag{A8}$$

$$|v_0\rangle = |u_1\rangle, \qquad |v_t\rangle = |v_{t+1}\rangle = \ldots = 0$$

$$\lambda_k^{(i)}(N) = \mathrm{O}(1), \qquad N \gg 1.$$

Proof. We may put

$$M_{ij}^{(m)} = \sum_{n-0}^{t-2} a_n^{(m)} (G^n)_{ij}$$

$$a_n^{(m+1)} = (-1)^{t+1} a_n^{(m)} + (-1)^{(t+1)m} a_n^{(1)} + \sum_{i=0}^{n-1} a_i^{(1)} a_{n-i-1}^{(m)}. \tag{A9}$$

Now, the element-by-element summations of the type $\Sigma m^k = \mathrm{O}(M^{k+1})$ imply that

$$a_n^{(m)} = \mathrm{O}(m^{n+1})$$

and the asymptotic expansion of (A6) in the powers of m

$$\gamma_m = |u_1\rangle a_{t-2}^{(m)} G_{1\,t-1}^{t-2} \langle v_{t-1}| + \sum_{\substack{(i,j)=(1,t-1),\\ (1,t-2)\\ (2,t-1)}} |u_i\rangle a_{t-1}^{(m)} G_{ij}^{t-1} \langle v_j| + \ldots$$

may be inserted into (5.10) to give

$$\gamma^{m\mathrm{T}} \gamma^m = |v_{t-1}\rangle (G_{1\,t-1}^{t-2} a_{t-2}^{(m)})^2 t \langle v_{t-1}| + \ldots$$

and

$$\frac{1}{\delta_N} = \text{constant } N^{2t-1} |v_{t-1}\rangle\langle v_{t-1}| + \ldots . \tag{A10}$$

Now, since $M_{ij}^{(m)} = \mathrm{O}(m^{j-i})$ for large $m \gg 1$, we may consider the non-orthogonal basis $|v_0\rangle (= |u_1\rangle), |v_1\rangle, \ldots, |v_{t-1}\rangle$ and invert the matrix

$$\left(\frac{1}{\delta_N}\right)_{ij} = m^{i/2} m^{j/2} \times \mathrm{O}(1)$$

to get $(\delta_N)_{ij} = m^{-i/2} m^{-j/2} \times \mathrm{O}(1)$. This coincides with the desired result after a slight re-arrangement.

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