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Schrödinger equation as recurrences: I. Band-matrix Hamiltonians

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Abstract. We describe a new algebraic treatment of the chain-model eigenvalue problem. It is based on the $(2t+1)$-diagonal and asymptotically smooth structure of the corresponding Hamiltonians. The formalism is illustrated on the phenomenological doubly anharmonic oscillators.

1. Introduction and summary

One of the most common formal difficulties connected with the applicability of perturbation theory is usually the lack of a suitable unperturbed Hamiltonian H_0. A textbook example is the anharmonic oscillator $H_\lambda = p^2 + r^2 + \lambda r^4$ where the obvious choice $H_0 = p^2 + r^2$ leads to divergences (Simon 1969).

The puzzling divergence of the anharmonic-oscillator energies E_λ may be removed easily by another choice of H_0 (Halliday and Suranyi 1980). Nevertheless, a more efficient solution of the Schrödinger eigenvalue problem $H_\lambda \psi = E_\lambda \psi$ was found by Graffi and Grecchi (1975). It employs directly the pentadiagonal structure of H_λ in the unperturbed oscillator basis, and represents the solution in terms of the matrix continued fractions (MCF).

In practice the MCF recurrent technique is formally applicable to any $(2t+1)$-diagonal Hamiltonian, i.e. to the so-called chain models appearing in various branches of physics (see e.g. Haydock (1980) and references therein). A simple testing example of such a system are the doubly anharmonic oscillators (DAHO)

$$\begin{aligned} &H_{(m,n)}\psi = E_{(m,n)}\psi, \\ &H_{(m,n)} = p^2 + r^2 + h_2 p^4 + g_2 r^4 + \ldots + h_m p^{2m} + g_n r^{2n}, \qquad h_m > 0,\ g_n > 0, \end{aligned} \tag{1}$$

investigated by Znojil (1981) and admitting various physical interpretations of the dispersive or 'velocity confining' anharmonicities $p^4 \ldots$ related originally to the semi-relativistic kinetic-energy operator $T(p) = (1+p^2)^{1/2} - 1 + \mathrm{O}(p^{2m+2})$.

When compared with some standard versions of perturbation theory, the non-numerical mathematical background of the MCF technique has been well developed for $t = 1$ only. Nevertheless, the general $t > 1$ MCF and chain models need not always be treated and interpreted in a semi-numerical context only. Our present intention is to show that some of the analytic $t = 1$ techniques may be generalised directly to any $t > 1$.

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The contents of our paper are organised as follows. In § 2 we review briefly the recurrent MCF idea. Its factorised reinterpretation (Znojil 1983) is recalled and applied to the Feshbach (1958) construction of the effective Hamiltonian in § 3.1. In § 3.2 this is illustrated on the simplest DAHO examples.

In the asymptotic 'quasiconstant' approximation, the elimination of recurrences and the general algebraic construction of ψ and underlying MCF quantities is obtained as our main result in §§ 4.1 and 4.2. Finally, in § 4.3, the symmetric DAHO example enables us to obtain closed analytic results including, e.g., the explicit $n \gg 1$ asymptotic behaviour of the wavefunctions.

We may summarise that the present method:

(1) clarifies algebraically the factorisable character of the multiterm recurrences and eigenvalue problem in the infinite-dimensional chain models,

(2) simplifies the rigorous analysis of the normalisability of ψ and also, in connection with the semi-numerical MCF technique, the proofs of the MCF convergence,

(3) provides a practical prescription how to construct the optimal and reliable 'smoothed' approximants to the band Hamiltonians in the purely numerical 'cut-off' context, and

(4) enables us to construct various algebraically invertible infinite auxiliary quasiconstant matrices H_0. As far as simplicity of the unperturbed basis is often preferred even to the smallness of the perturbations $H-H_0$, this might help us to achieve suitable rearrangements of perturbation theory (cf e.g. Znojil 1980) and/or to understand its divergences in the future.

2. The Feshbach and MCF methods

In the general infinite-dimensional linear equation of the non-homogeneous or Schrödinger type,

$$H\psi = E\psi + \chi, \tag{2}$$

we shall consider a non-zero or zero input function χ such that $\chi = P\chi$, where P denotes a finite-dimensional projector on a 'model' subspace of the whole Hilbert space. It is useful to partition (2) and write

$$P(H-E)P\psi + PHQ\psi = P\chi, \qquad Q = 1-P, \qquad QHP\psi + Q(H-E)Q\psi = 0.$$

Formally we may eliminate $Q\psi[=(E-QHQ)^{-1}QHP\psi]$ from the second row and obtain the first one in a simple form

$$\mathscr{H}(E)\varphi = \chi. \tag{3}$$

With $\varphi = P\psi$ and with the definition

$$\mathscr{H}(E) = P(H-E)P - PHQ[Q(H-E)Q]^{-1}QHP \tag{4}$$

of the finite-dimensional 'effective' matrix Hamiltonian, this is the essence of the projection method of Feshbach (1958).

Obviously, equation (3) may be solved numerically with arbitrary precision. As a finite-dimensional inversion or eigenvalue problem (with $\chi \neq 0$ or $\chi = 0$, respectively) it disguises all the infinite-dimensional algebra of (2) in the definition (4).

In the following text, we shall assume that the operator H has a block-tridiagonal structure in the chosen basis,

$$H-EI=\begin{pmatrix} A_0 & B_0 & & \\ C_1 & A_1 & B_1 & \\ & C_2 & A_2 & B_2 \\ & & \ldots & \end{pmatrix}, \qquad \dim A_k = t, \qquad k=0,1,\ldots. \tag{5}$$

As a consequence, definition (4) leads to the partitioned form of the effective Hamiltonians

$$\mathscr{H}(E)=\mathscr{H}_{(k)}(E)=\begin{pmatrix} A_0 & B_0 & & \\ & \ldots & & \\ & C_{k-1} & A_{k-1} & B_{k-1} \\ & & C_k & G_k \end{pmatrix} \tag{6}$$

where $P=|0\rangle\langle 0|+|1\rangle\langle 1|+\ldots+|(k+1)t-1\rangle\langle (k+1)t-1|$ and

$$G_k=A_k-B_kG_{k+1}^{-1}C_{k+1}, \qquad k=0,1,\ldots. \tag{7}$$

In agreement with Znojil (1980), the MCF recurrences (7) may be initialised by the truncation of H, namely, by $G_N=A_N$ in the limit $N\to\infty$. This completes the reduction of (2) to its finite-dimensional equivalent (3).

3. Chain models and exact effective Hamiltonians

In agreement with § 2, the correct MCF input (exact effective $(t\times t)$-dimensional submatrix G_k) reduces (2) to the trivial equation (3) and *vice versa*, any linear problem (2) with the band matrix Hamiltonian H leads in essence to the infinite-dimensional inversion of $Q(H-E)Q$. Thus, we may replace recurrences (7) by the rigorous non-MCF definition

$$G_k=P_k\frac{1}{P_k\dfrac{1}{R_k(H-E)R_k}P_k}P_k \tag{8}$$

written in terms of the projectors

$$P_k=|kt\rangle\langle kt|+|kt+1\rangle\langle kt+1|+\ldots+|(k+1)t-1\rangle\langle (k+1)t-1|,$$

$$R_{k+1}=I-P_0-P_1-\ldots-P_k, \qquad k\geqslant 0, R_0=I.$$

3.1. *Complete factorisation*

Assuming for simplicity that the matrices B_k and C_{k+1}^{T} in (5) are lower triangular, we may evaluate directly the projected inversion $P_k[R_k(H-E)R_k]^{-1}P_k$ in (8) by means of the complete factorisation method (Znojil 1983). In essence, this method is based on the decomposition of $H-EI$ into the product

$$H-EI=\begin{pmatrix}\rho_1 & & \\ & \rho_2 & \\ & & \ddots\end{pmatrix}\times K_{\mathrm{U}}\times\begin{pmatrix}\gamma_1 & & \\ & \gamma_2 & \\ & & \ddots\end{pmatrix}\times K_{\mathrm{L}}\times\begin{pmatrix}\sigma_1 & & \\ & \sigma_2 & \\ & & \ddots\end{pmatrix}, \tag{9}$$

$$K_{\mathrm{U}}=\prod_{i=1}^{t}\begin{pmatrix}1 & \alpha_1^{(i)} & 0 & \dots & \\ 0 & 1 & \alpha_2^{(i)} & 0 & \dots\\ 0 & 0 & 1 & \alpha_3^{(i)} & \\ & & & \dots & \end{pmatrix},\qquad K_{\mathrm{L}}=\prod_{j=1}^{t}\begin{pmatrix}1 & 0 & \dots & & & \\ \beta_1^{(j)} & 1 & 0 & \dots & & \\ 0 & \beta_2^{(j)} & 1 & 0 & \dots & \\ \dots & & & & & \end{pmatrix},$$

of the $2t$ two-diagonal and 3-diagonal auxiliary matrices. In our original paper, the detailed algebraic recurrent definitions of the quantities ρ_n, $\alpha_n^{(i)}$, γ_n, $\beta_n^{(j)}$ and σ_n ($i, j=1, 2, \dots, t$, and $n=1, 2, \dots$) were studied, while here we re-emphasise only their standard initialisation (with $(H)_{M+i,M+j}=0$, $i, j=1, 2, \dots$ in the 'cut-off' limit $M\to\infty$) and prove the following.

Theorem 1. For the factorised Hamiltonians (9), we may write formally their explicit Feshbach $(N\times N)$-dimensional equivalents in the form (6) with $N=(k+1)t$ and with the effective $(t\times t)$-dimensional submatrices

$$G_k=\begin{pmatrix}\rho_{N-t+1} & & \\ & \ddots & \\ & & \rho_{N-1} & \\ & & & \rho_N\end{pmatrix}\times\prod_{i=1}^{t}\begin{pmatrix}1 & \alpha_{N-t+1}^{(i)} & & \\ & \dots & & \\ & & 1 & \alpha_{N-1} \\ & & & 1\end{pmatrix}\times\begin{pmatrix}\gamma_{N-t+1} & & & \\ & \ddots & & \\ & & \gamma_{N-1} & \\ & & & \gamma_N\end{pmatrix}$$

$$\times\prod_{j=1}^{t}\begin{pmatrix}1 & & \\ \beta_{N-t+1}^{(j)} & 1 & \\ \dots & & \\ & \beta_{N-1}^{(j)} & 1\end{pmatrix}\times\begin{pmatrix}\sigma_{N-t+1} & & & \\ & \sigma_{N-t+2} & & \\ & & \ddots & \\ & & & \sigma_N\end{pmatrix}. \tag{10}$$

Proof. The product form of (9) enables us to write any projection of $H-E$ as the same projected product of the two-diagonal factors. Thus we get (10) after the double use of the formula

$$\begin{pmatrix}1 & \delta_1 & \\ & 1 & \delta_2 \\ & \dots & \end{pmatrix}^{-1}=\begin{pmatrix}1 & -\delta_1 & \delta_1\delta_2 & \dots \\ & 1 & -\delta_2 & \dots \\ & & \dots & \end{pmatrix} \tag{11}$$

in (8).

3.2. *Example: asymmetric* DAHO

In the oscillator basis, the phenomenological DAHO Hamiltonians $H=H_{(m,n)}$ in (1) have a symmetric and real band-matrix form with $2t+1$ diagonals, $t=\max(m, n)$. From the formal point of view it is convenient to consider a large index k in (6).

Then we may replace the complicated DAHO matrix elements by their asymptotic expansions. In the leading order, we get the formula

$$
\begin{aligned}
Q(H-E)Q &= g_n N^n K(1+\mathrm{O}(1/N)), && m<n,\\
&= h_m N^m JKJ(1+\mathrm{O}(1/N)), && m>n
\end{aligned}
\tag{12}
$$

$$
N=(k+1)t, \qquad Q=R_{k+1}, \qquad J=\begin{pmatrix} -1 & & & \\ & 1 & & \\ & & -1 & \\ & & & \ddots \end{pmatrix},
$$

where K is a constant matrix such that

$$
K=\prod_{i=1}^{t} I_{(+)}\times\prod_{j=1}^{t} I_{(+)}^{\mathrm{T}}, \qquad I_{(+)}=\begin{pmatrix} 1 & 1 & & & \\ & 1 & 1 & & \\ & & 1 & 1 & \\ & & & & \ldots \end{pmatrix}. \tag{13}
$$

Hence, we may apply theorem 1 and obtain immediately the effective matrix Hamiltonian $\mathscr{H}(E)$ and equation (3) in the leading-order approximation.

Below we shall use also the symmetric ($m=n$) DAHO chain model as another illustrative example. Due to the exact elimination of its outer diagonal in some bases, its factorisation will be much less trivial.

4. Asymptotically smooth chain models

In the following, we shall assume that $Q(H-E)Q$ may be approximated by a constant matrix K (cf example (12)) or by a product $\rho K\sigma$ where ρ and σ are some appropriate diagonal matrices introduced in (9), reflecting, e.g., the overall increase of matrix elements with increasing indices, and containing possibly also the error estimates of the type $1+\mathrm{O}(1/N)$, $N=\dim P$, $P=1-Q$. Formally, the presence of ρ and σ is irrelevant—we may include σ in the 'renormalised' vector, $\psi\to\sigma\psi$, and simply multiply equation (1) by the non-singular factor ρ^{-1} from the left.

4.1. Algebraic factorisation of K

In the real and symmetric case, the factorisation (9) of the constant matrix K may be given the form

$$
\begin{aligned}
K &= \begin{pmatrix} a_t(t), & a_{t-1}(t), & \ldots & a_0(t), & 0, & \ldots & & \\ a_{t-1}(t), & a_t(t), & a_{t-1}(t), & \ldots & a_0(t), & 0, & \ldots \\ \ldots & & & & & & \end{pmatrix} \\
&= \gamma\times K_{\mathrm{U}}\times K_{\mathrm{L}},
\end{aligned}
\tag{14}
$$

$$
\begin{aligned}
K_{\mathrm{U}} &= \begin{pmatrix} 1 & \alpha^{(1)} & 0 & \ldots & \\ 0 & 1 & \alpha^{(1)} & 0\ldots \\ & & \ldots & \end{pmatrix}\times\begin{pmatrix} 1 & \alpha^{(2)} & 0 & \ldots & \\ 0 & 1 & \alpha^{(2)} & 0 & \ldots \\ & & \ldots & & \end{pmatrix} \\
&\quad\ldots\times\begin{pmatrix} 1 & \alpha^{(t)} & 0 & \ldots & \\ 0 & 1 & \alpha^{(t)} & 0 & \ldots \end{pmatrix}=K_{\mathrm{L}}^{\mathrm{T}},
\end{aligned}
$$

with the constant diagonal matrix, $\gamma = 1/(\alpha^{(1)}\alpha^{(2)}\ldots\alpha^{(t)})$; with the normalisation of matrix elements $a_0(t) = 1$, and with the mutually commutative two-diagonal factors in K_U. Our intention is to illustrate the general factorisation method of § 3 by its application to the specific matrices (14), i.e., in essence, to define the matrix elements $\alpha^{(1)}, \alpha^{(2)}, \ldots, \alpha^{(t)}$ as functions of $a_1(t), a_2(t), \ldots, a_t(t)$ in an explicit way.

In the simplest $t = 1$ case, we have $a_1(1) = \alpha^{(1)} + 1/\alpha^{(1)}$ with an elementary inversion. The first non-trivial $t = 2$ example

$$a_1(2) = \alpha^{(1)} + 1/\alpha^{(1)} + \alpha^{(2)} + 1/\alpha^{(2)},$$

$$a_2(2) = 2 + (\alpha^{(1)} + 1/\alpha^{(1)})(\alpha^{(2)} + 1/\alpha^{(2)}),$$

inspires us to eliminate the irrelevant $\alpha \to 1/\alpha$ ambiguity and to denote $\alpha^{(i)} = \exp(\pm\beta_i)$ or, with $2\cosh\beta_i = X_{(i)}$,

$$\alpha^{(i)} = \alpha^{(i)}_{(\pm)} = \tfrac{1}{2}X_{(i)} \pm (\tfrac{1}{4}X^2_{(i)} - 1)^{1/2}. \tag{15}$$

In general, we then have the following theorem.

Theorem 2. Factorisation (9) of the constant matrix K may be defined by formulae (14) and (15) where the factors $X_{(i)}$ are roots of the polynomial equation

$$\sum_{k=0}^{t} (-1)^k T_k(a) X^{t-k} = 0 \tag{16}$$

and

$$T_k(a) = \sum_{j=0}^{[k/2]} (-1)^j \binom{t-k+j}{j}\left(1 + \frac{j}{t-k+j}\right) a_{k-2j}(t)$$

are linear functions of the matrix elements of K.

Proof. From the recurrences (14), i.e.

$$a_0(t) = 1,$$

$$a_1(t) = 2\cosh\beta_1 + 2\cosh\beta_2 + \ldots + 2\cosh\beta_t,$$

$$\ldots$$

$$a_k(t) = a_k(t-1) + 2\cosh\beta_t a_{k-1}(t-1) + a_{k-2}(t-1),$$

$$\ldots$$

$$a_t(t) = 2\cosh\beta_t a_{t-1}(t-1) + 2a_{t-2}(t-1),$$

we infer a possibility to use the ansatz

$$a_k(t) = \sum_{j=0}^{[k/2]} A_j^{(k)}(t) \sum_{\{i_j\}} \cosh\beta_{i_1}\cosh\beta_{i_2}\ldots\cosh\beta_{i_{k-2j}} \tag{17}$$

for any $t \geq 1$. The unknown coefficients $A_j^{(k)}(t)$ may be obtained from the recurrences (14) by insertion. It is documented in table 1 and illustrated by the further $t = 3$ example

$$a_0(3) = 1,$$

$$a_1(3) = 2\cosh\beta_1 + 2\cosh\beta_2 + 2\cosh\beta_3,$$

$$a_2(3) = 3 + 4(\cosh\beta_1\cosh\beta_2 + \cosh\beta_1\cosh\beta_3 + \cosh\beta_2\cosh\beta_3),$$

$$a_3(3) = 2a_1(3) + 8\cosh\beta_1\cosh\beta_2\cosh\beta_3.$$

Now our task is to define the inverse mapping $a_j \to \beta_i$, $1 \leq i, j \leq t$.

Table 1. Sample of coefficients $A_j^{(k)}(t)$.

k \ j	0	1	2	3
0	1			
1	2			
2	4	t		
3	8	$2(t-1)$		
4	16	$4(t-2)$	$\binom{t}{2}$	
5	32	$8(t-3)$	$2\binom{t-1}{2}$	
6	64	$16(t-4)$	$4\binom{t-2}{2}$	$\binom{t}{3}$
7	128	$32(t-5)$	$8\binom{t-3}{2}$	$2\binom{t-1}{3}$

Our first result concerns the compact and explicit formula

$$A_j^{(k)}(t) = 2^{k-2j}\binom{t-k+2j}{j} \tag{18}$$

which may be verified by mathematical induction and a certain amount of patient elementary manipulations. As a consequence, the mapping (17) may be reinterpreted as a composition of nonlinear transformations $\cosh\beta_k \to S_i$ $(\cosh\beta_1, \ldots, \cosh\beta_t)$ with a pair of two separate linear mappings

$$a_{2i}(t) = \sum_{k=0}^{i}\binom{t-2k}{i-k}4^k S_{2k}(\cosh\beta_1, \cosh\beta_2, \ldots, \cosh\beta_t), \qquad i = 1, 2, \ldots, [t/2], \tag{19}$$

and

$$a_{2i-1}(t) = \sum_{k=1}^{i}\binom{t-2k+1}{i-k}2^{2k-1}S_{2k-1}(\cosh\beta_1, \cosh\beta_2, \ldots, \cosh\beta_t), \tag{20}$$

$$i = 1, 2, \ldots, [(t+1)/2],$$

where

$$S_0(x_1, x_2, \ldots, x_n) = 1, \qquad S_1(x_1, x_2, \ldots, x_n) = x_1 + x_2 + \ldots + x_n, \ldots,$$
$$S_n(x_1, x_2, \ldots, x_n) = x_1 x_2, \ldots, x_n, \tag{21}$$

are the ordinary symmetric functions defined by the identity

$$\sum_{m=0}^{N} x^{N-m} S_m(x_1, x_2, \ldots, x_N) = \prod_{i=1}^{N}(x + x_i). \tag{22}$$

The matrices of the linear systems (19) and (20) are triangular and easily invertible (appendix). Hence, we may also invert the mapping $a_i(t) \leftarrow S_j$,

$$S_m(\cosh\beta_1, \ldots, \cosh\beta_t) = 2^{-m}T_m(a), \qquad m = 0, 1, \ldots, t. \tag{23}$$

Finally, the definition (22) of the symmetric functions S_m implies that the polynomial equation

$$\sum_{m=0}^{t} (-1)^m 2^{-m} T_m(a)(\cosh\beta)^{t-m} = 0$$

determines all the factors $\alpha^{(i)}$ in (14) in a purely algebraic way.

4.2. *Wavefunctions*

Obviously, in terms of the β or X variables defined by theorem 2, the purely algebraic definition of the asymptotic effective Hamiltonian (6) is an easy consequence of theorem 1. Nevertheless, rather surprisingly, the matrix elements of K^{-1} are not unique in general. For example, we get $G_k^{(1)} = 1/\alpha_{(+)}^{(1)}$ and $G_k^{(2)} = 1/\alpha_{(-)}^{(1)} = \alpha_{(+)}^{(1)}$ for $t = 1$.

This ambiguity is not encountered in the asymptotic $m \neq n$ DAHO examples (12) where $\alpha_{(\pm)}^{(i)} = 1$, $i = 1, 2, \ldots, t$. In the other, non-degenerate chain models, we may prove the following.

Theorem 3. Provided that $\sigma_k/\sigma_{k-1} = 1 + O(1/k)$, $k \gg 1$, and $X_{(i)} > 2$, $X_{(i)} \neq X_{(j)}$, $i, j = 1, 2, \ldots, t$, the norm of the wavefunctions.

$$\|\psi\| = \left(\sum_{n=0}^{\infty} \langle\psi|n\rangle\langle n|\psi\rangle \right)^{1/2},$$

is finite if and only if we choose $\alpha^{(i)} = \alpha_{(-)}^{(i)}$ in (15).

Proof. Since $|\alpha_{(+)}^{(i)}| > 1$ and $|\alpha_{(-)}^{(i)}| < 1$, we may neglect the higher-order corrections and write the definitions

$$QKQ\psi = -QKP\psi = \begin{pmatrix} c_1 \\ \vdots \\ c_t \end{pmatrix},$$

$$Q\psi = \frac{1}{QKQ} \begin{pmatrix} c_1 \\ \vdots \\ c_t \end{pmatrix} = K_L^{-1} K_U^{-1} \begin{pmatrix} c_1 \\ \vdots \\ c_t \end{pmatrix} = K_L^{-1} \begin{pmatrix} d_1 \\ \vdots \\ d_t \end{pmatrix}$$

$$= \begin{pmatrix} 1 & & & & \\ -\alpha^{(1)} - \alpha^{(2)} - & \cdots & -\alpha^{(t)} & 1 \\ \cdots & & & \end{pmatrix} \begin{pmatrix} d_1 \\ \vdots \\ d_t \end{pmatrix}.$$

Here, the explicit form of the matrix elements may be inserted, which gives

$$\langle N + m - 1|\psi\rangle = \sum_{k=1}^{\min(m,t)} (-1)^{k+m} d_k \sum_{i=1}^{t} \frac{(\alpha^{(i)})^{m+t-k-1}}{\prod_{j \neq i} (\alpha^{(i)} - \alpha^{(j)})}, \qquad m = 1, 2, \ldots. \tag{24}$$

This is one of our most interesting formulae and implies that, for $m \gg 1$, we have an estimate

$$|\langle m|\psi\rangle / \langle m-1|\psi\rangle| \doteq \max_{1 \leq i \leq t} |\alpha^{(i)}|, \qquad m \gg 1. \tag{25}$$

Hence, the infinite series $\|\psi\|$ converges or diverges as a geometric series.

To avoid confusion, we must re-emphasise that the above energy-independent construction of the normalisable vector ψ is not contradictory since this vector satisfies the Schrödinger equation at the physical energies only.

4.3. Example: symmetric DAHO

After an appropriate scaling of coordinates $r \to \nu r$, $p \to (1/\nu)p$, an approximate cancellation of diagonals in the DAHO $m = n$ matrix $H_{(m,n)ij}$ may be achieved in the $i, j \gg 1$ asymptotic region. Thus, instead of (12), we get the leading-order formula

$$H_{(m,n)ij} - E\delta_{ij} = \rho_i \tilde{K}_{ij} \sigma_j, \qquad i, j \gg 1, \tag{26}$$

$$\delta_{ij} \begin{matrix} = 1, & i = j \\ = 0, & i \neq j \end{matrix}, \qquad \tilde{K}_{ij} = \binom{2m}{m + i - j} \pi_{ij},$$

$$\pi_{ij} \begin{matrix} = 1, & |i - j| = \text{even}, \\ = 0, & |i - j| = \text{odd}, \end{matrix}$$

where ρ_i and σ_i contain again the irrelevant i and j dependence of H_{ij} and possibly also the explicit non-diagonal error estimates $1 + O(1/(i + j))$.

The factor π_{ij} is a projector on the even- or odd-indexed subspaces so that it is sufficient to consider just one of the two orthogonal and identical infinite matrices K with the smaller parameter $t = t_{as} =$ integer part of $(\frac{1}{2}m)$. Thus with the matrix elements

$$K_{ij} = \binom{2m}{m + 2i - 2j}, \qquad i, j = 1, 2, \ldots, \tag{27}$$

we may use theorems 1 and 2.

One of the most obvious ways to eliminate the $\alpha \to 1/\alpha$ ambiguity without any recourse to theorem 3 is to return to the original MCF interpretation of G_k. We do not get any contradiction—in the simplest quartic–quartic example with $m = n = 2t_{as} = 2$, the continued-fractional result

$$G_k \sim 6 - \cfrac{1}{6 - \cfrac{1}{6 - \ldots}} = 3 + 2\sqrt{2} \doteq 5.828 \tag{28}$$

is easily summable and eliminates the plus-sign choice in (15). Similarly, for $m = n = 3$, we get $t_{as} = 1$ and

$$G_k \sim 20/6 - \cfrac{1}{20/6 - \cfrac{1}{20/6 - \ldots}} = 3. \tag{29}$$

Starting from $m = n = 4$, the corresponding algebra may be combined with the numerical tests as well.

In the light of theorem 3, criterion (25) specifies now the upper $P\psi$-independent estimate of the rate of convergence of $\|\psi\|$. Up to the sufficiently high-order potentials $V = H_{(m,n)} - p^2 \sim p^{18} + \ldots + r^{18}$ with $t_{as} \leqslant 4$, this is still a non-numerical task in principle—we may obtain $\alpha^{(i)}$ by algebraic means. For convenience, the corresponding $t \leqslant 4$ linear functions $T_k(a)$ to be used in (16) are listed here in table 2.

In table 3 the explicit exact values of cosh β_i are given up to the duodecadic–duodecadic DAHO case. We may notice that the assumptions of theorem 3 appear to be satisfied so that, in contrast to the asymmetric DAHO examples, the corresponding

Table 2. First five functions $T_t(a) = 2^t S_i(\cosh\beta_1, \ldots, \cosh\beta_t)$.

$T_0(a) = 1$	$t \geqslant 0$
$T_1(a) = a_1$	$t \geqslant 1$
$T_2(a) = a_2 - t$	$t \geqslant 2$
$T_3(a) = a_3 - (t-1)a_1$	$t \geqslant 3$
$T_4(a) = a_4 - (t-2)a_2 + t(t-3)/2$	$t \geqslant 4$

Table 3. Leading-order asymptotic factorisation of the symmetric DAHO operator $H = p^{2m} + \ldots + r^{2m}$.

m	i	$\frac{1}{2}X_{(i)}$	$\alpha^{(1)}$
2	1	3	0.171 572 875 ...
3	1	5/3	0.333 333 333 ...
4	1	$7+4\sqrt{2}$	0.039 566 129 ...
	2	$7-4\sqrt{2}$	0.446 462 692 ...
5	1	$3+4/\sqrt{5}$	0.105 572 808 ...
	2	$3-4/\sqrt{5}$	0.527 864 045 ...
6	1	$15+8\sqrt{3}$	0.017 332 380 ...
	2	3	0.171 572 875 ...
	3	$15-8\sqrt{3}$	0.588 790 706 ...

wavefunctions lie mostly within a small model space. Also the norm $\|\psi\|$ converges extremely quickly. All these features of the symmetric DAHO system are compatible with the preceding numerical results (Znojil 1981).

Appendix. Inversion of the triangular matrices

For the triangular matrices

$$\begin{pmatrix} 1 & & & \\ a_1 & 1 & & \\ b_1 & a_2 & 1 & \\ c_1 & b_2 & a_3 & 1 \\ \ldots & & & \end{pmatrix} \tag{A1}$$

the inverse

$$\begin{pmatrix} 1 & & \\ \alpha_1 & 1 & \\ \beta_1 & \alpha_2 & 1 \\ \ldots & & \end{pmatrix} \tag{A2}$$

is defined by the obvious relations

$$\begin{aligned} &a_i + \alpha_i = 0, \qquad b_i + a_{i+1}\alpha_i + \beta_i = 0, \\ &c_i + b_{i+1}\alpha_i + a_{i+2}\beta_i + \gamma_i = 0, \qquad \ldots, \qquad i = 1, 2, \ldots, \end{aligned} \tag{A3}$$

and it may be given the explicit Kramer form (Korn and Korn 1968)

$$\alpha_i = -\det(a_i), \qquad \beta_i = +\det\begin{pmatrix} a_i & 1 \\ b_i & a_{i+1} \end{pmatrix}, \tag{A4}$$

$$\gamma_i = -\det\begin{pmatrix} a_i & 1 & 0 \\ b_i & a_{i+1} & 1 \\ c_i & b_{i+1} & a_{i+2} \end{pmatrix}, \qquad \ldots$$

In particular, for the matrix elements (18),

$$a_i = \binom{T-2i+2}{1}, \qquad b_i = \binom{T-2i+2}{2}, \qquad c_i = \binom{T-2i+2}{3}, \qquad \ldots, \tag{A5}$$

we may evaluate (A4)

$$\begin{aligned} &\alpha_i = -(T-2i+2), \qquad \beta_i = +\tfrac{1}{2}(T-2i+2)(T-2i-1), \\ &\gamma_i = -\tfrac{1}{6}(T-2i+2)(T-2i-2)(T-2i-3), \qquad \ldots, \end{aligned} \tag{A6}$$

and, changing the notation to

$$\alpha_i = B_i^{(1)}(T), \qquad \beta_i = B_i^{(2)}(T), \qquad \gamma_i = B_i^{(3)}(T), \ldots,$$

we arrive at the final formula

$$B_i^{(k)}(T) = (-1)^k \frac{T-2i+2}{T-2i+2-k}\binom{T-2i-k+2}{k}, \qquad i = 1, 2, \ldots, \tag{A7}$$

which defines the integer coefficients needed in (19) and (20) in § 4.1.

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