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The recursion method of a linear operator inversion II

M Znojil†

Institute for Nuclear Research, Soviet Academy of Sciences, Moscow, USSR

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Abstract. In the second part of the present series we describe the sparse-matrix version of the Born series generalisation.

1. Introduction

In paper I (Znojil 1976), we investigated the generalised power series expansion of the resolvent operator $\hat{R}(E) = (E - \hat{H})^{-1}$ inspired by Haydock (1974) and not employing any scalar product definition. It was based on the parametrisation of action \hat{H} on the vector $|X_1\rangle \in \kappa$, the parameters being considered elements of a Hessenberg matrix Q . Appropriate linear combinations of the vectors $|X_1\rangle, \hat{H}|X_1\rangle, \dots, \hat{H}^k|X_1\rangle$ with the coefficients constructed by means of the matrix Q were denoted as $|X_k\rangle$. Intended to be as simple and 'non-numerical' as possible, they represented an adequate set for expansion of the vectors $|Y_k\rangle = \hat{R}(E)|X_k\rangle, k \geq 1$.

Later (Znojil 1977, denoted as Ia) we suggested another parametrisation of this type employing Q in the quasitridiagonal (block-tridiagonal) form. Further generalisation of Q was not investigated at the time because of an abrupt increase in complexity of the general formulae for $|Y_k\rangle, k > 1$.

Fortunately, the practical calculations rarely demand the full knowledge of the operator $\hat{R}(E)$. Since the next generalisation using the quasi-Hessenberg Q would be best suited to the construction of 'non-numerical' vectors $|X_k\rangle$, we accept this form in the present paper while restricting our attention to the expansion of $\hat{R}(E)$ acting on some finite group of vectors $|X_1^1\rangle, |X_1^2\rangle, \dots, |X_1^{M_1}\rangle$ only. It will be shown that due to this restriction, the resulting formulae preserve the simplicity of the previous versions of the method, especially the use of only one infinite ($N \rightarrow \infty$) auxiliary sequence $F_k(E), k = N, N-1, N-2, \dots, 1$, calculated in a recurrent way (§2).

The choice of the free parameters Q is quite arbitrary—hence the flexibility of the method. The required knowledge of \hat{H} is minimal—it concerns its action on suitable $|X_1^i\rangle$'s and does not embody scalar product, orthogonality or any properties of the conjugated operator \hat{H}^+ . Hence, the iteration represents in general the only possible test of convergence. It is of fundamental importance that such a test may be performed within the framework of the formalism (§3). In addition, some important relations between convergence and the spectral properties of \hat{H} and Q are illustrated in appendix 1.

† Present address: Institute of Nuclear Physics, Czechoslovak Academy of Sciences, CS 250 68 Rez, Czechoslovakia.

An important feature of the method is the double indexing of the expansion set $|X_k^m\rangle$, $m = 1, 2, \dots, M_k < \infty$, $k = 1, 2, \dots, N$, $N \rightarrow \infty$ with variable M_k (the number of vectors in the k th subset or partition). This is important in the applications: in §4, we illustrate this by the quick and exact evaluations of the matrix elements of Köhler's kernel of the Bethe–Goldstone equation used in the Brueckner theory of finite nuclei. At the same time, this example shows how any sparse matrix \hat{H} (having finite number of non-zero elements in each row) may be related to the quasi-Hessenberg Q (and only to this form in general) by a simple permutation of the basis.

There are always restrictions on applicability of any method. Here, together with the points of the spectrum of \hat{H} , we must avoid another set of 'dangerous' values of E . There are two ways of doing this discussed in appendix 2.

2. The method

Let us assume that we have the set of M_1 initial states $|X_1^i\rangle \in \kappa$, $i = 1, 2, \dots, M_1$ such that the action of \hat{H} on them is given as finite linear superposition

$$\hat{H}|X_1^i\rangle = \sum_{j=1}^{M_1} |X_1^j\rangle A_1^{ij} + \sum_{j=1}^{M_2} |X_2^j\rangle B_1^{ij} \tag{1}$$

employing another M_2 simple states $|X_2^i\rangle \in \kappa$, $i = 1, 2, \dots, M_2$. The freedom in the choice of coefficients A_1^{ij} , B_1^{ij} ($M_2 \neq M_1$) is intended to enable us to repeat the introduction of new and simple states in a recurrent way,

$$\hat{H}|X_k^i\rangle = \sum_{j=1}^{M_k} |X_k^j\rangle A_k^{ij} + \sum_{j=1}^{M_{k+1}} |X_{k+1}^j\rangle B_k^{ij} + \sum_{l=1}^{p(k)} \sum_{j=1}^{M_l} |X_l^j\rangle C_{k(k-l)}^{ij},$$

$$p(k) \leq k - 1, k \geq 1. \tag{2}$$

Since we do not want to employ orthogonality of $|X\rangle$'s, all C 's may be non-zero even for the Hermitian \hat{H} . For $p(k) = 1$ and $M_k = M_{k+1} = M$, formula (2) coincides with the definition given in Ia. For $p(k) = k - 1$ and $M_k = 1$, we arrive at the method of I.

In order to keep the structure of formulae as clear as possible, we simplify slightly the notation omitting the upper indices in $|X_k^i\rangle$, A_k^{ij} , ... and assuming the summation conventions of usual matrix multiplication. Formula (2) may thus be written as

$$\hat{H}|X_k\rangle = \sum_j Q_{kj}|X_j\rangle = \sum_j |X_j\rangle Q_{jk}^T \tag{3}$$

where the (partitioned) matrix Q is composed of blocks A , B , C . In this way, intertwining (3) and the product decomposition

$$Q - EI = \begin{pmatrix} A_1 - EI & B_1 & 0 & \dots \\ C_{2(1)} & A_2 - EI & B_2 & 0 \dots \\ \vdots & & & \\ C_{N(N-1)} & C_{N(N-2)} & \dots \\ \vdots & & & \end{pmatrix}$$

$$= \begin{pmatrix} I & L_1 & 0 & \dots \\ 0 & I & L_2 & 0 \dots \\ \vdots & & & \\ 0 & \dots & & \\ \vdots & & & \end{pmatrix} \times \begin{pmatrix} U_{1(0)} & 0 & \dots \\ U_{2(1)} & U_{2(0)} & 0 \dots \\ \vdots & & \\ U_{N(N-1)} & \dots & \\ \vdots & & \end{pmatrix} \tag{4}$$

form the fundamental idea of the present method—the initialisation $L_N = 0$, $U_{N(0)} = A_N - EI$ and the recurrence relations

$$\begin{aligned} U_{j(i)} &= C_{j(i)} - L_j U_{j+1(i+1)}, & i &= 1, 2, \dots, j-1, \\ L_{j-1} &= B_{j-1} U_{j(0)}^{-1}, & & \\ U_{j-1}(0) &= A_{j-1} - EI - L_{j-1} U_{j(1)}, & j &= N, N-1, \dots, 2 \end{aligned} \tag{5}$$

define the unknown quantities in (4) for $N \rightarrow \infty$. The serious question of existence and uniqueness of the limit $N \rightarrow \infty$ is not discussed here because it depends on the more specific assumptions about Q which will not be considered here (cf I).

Let us formally proceed in analogy with I, Ia. We define the general expansion of $\hat{R}(E)$ in the form of an *ansatz*

$$|Y_k^m\rangle = \hat{R}(E)|X_k^m\rangle = \sum_{r=1}^{\infty} \sum_{n=1}^{M_r} |X_r^n\rangle D_{(k)r}^{mn} \tag{6}$$

that is,

$$|Y_k\rangle = \sum_{r=1}^{\infty} D_{(k)r} |X_r\rangle \tag{6a}$$

and obtain the set of (matrix) equations

$$\begin{aligned} \delta_{kl}I &= D_{(k)l}(EI - A_l) - D_{(k)l-1}B_{l-1} - \sum_{i=1}^{\infty} D_{(k)l+i}C_{l+i(i)} \\ \delta_{kl}I &= (EI - A_k)D_{(k)l} - B_k D_{(k+1)l} - \sum_{i=1}^{k-1} C_{k(k-i)}D_{(i)l} \end{aligned} \tag{7}$$

for the expansion coefficients connected with the submatrices of $(E - Q)^{-1}$ in an obvious way.

We intend to solve (7) in terms of only one infinite ($N \rightarrow \infty$) matrix sequence $F_k(E) = -U_{k(0)}^{-1}$. It is easy to verify that this fundamental sequence is defined (cf (5) and I, Ia) by the matrix recurrence formula

$$F_j(E) = \left(EI - A_j - \sum_{i=1}^{\infty} (B_j F_{j+1} B_{j+1} F_{j+2} \dots B_{j+i-1} F_{j+i}) C_{j+i(i)} \right)^{-1} \tag{8}$$

with j decreasing from infinity to one. In practice, the dimension cut-off is assumed. For the initialisation

$$F_{N+1}(E) = F_{N+2}(E) = \dots = 0 \tag{9}$$

we shall write $F_k(E) = F_k(E, N)$ and assume again the limit $N \rightarrow \infty$ to be well defined.

Here, the completeness of analogy with I, Ia breaks down—we do not have the matrices B_k^{-1} at our disposal and the full and closed solution of (7) for $N \rightarrow \infty$ may

therefore be defined in terms of the set of infinite sequences $U_{k(1)}, U_{k(2)}, \dots$ only. It may be shown that using F_k 's, we may define by a finite number of operations the solutions $D_{(k)j}$ of (7) for $k = 1$ only. In this case, we obtain the partial result, expansion (6) of $|Y_1^m\rangle$, $m = 1, 2, \dots, M_1$ with

$$D_{(k)l} = D_{(k)l-1}B_{l-1}F_l, \quad l > k, \quad D_{(1)1} = F_1 \tag{10}$$

equivalent to I or Ia. With respect to the variability of M_1 , this is in fact all we need in practice. When using the finite cut-off N (initialisation (9) of $F_k(E, N)$), we denote also $D_{(k)j}(E) = D_{(k)j}(E, N)$ in (10).

3. The iterative prescription

The restricted solvability of (7) in terms of the sequence F_k may be understood by realising that the iterated use of (2) defines uniquely M_k vectors $B_k|X_{k+1}\rangle$ only: for $M_{k+1} > M_k$, the specific choice of separate $M_{k+1} - M_k$ vectors $|X_{k+1}^i\rangle$ is arbitrary, and hence also the very definition of $\hat{R}(E)|X_{k+1}\rangle$ and $\bar{D}_{(k+1)j}$.

In this sense, we may try to solve the set of equations (7) in terms of F_k 's for the appropriately 'dimension-reduced' matrices of the form $\Theta_k D_{(k+1)j}$ choosing the simplest matrices Θ_k which allow such a solution. After straightforward though rather lengthy algebra we obtain the result

$$\begin{aligned} \Theta_k &= D_{(1)k}(E, k)B_k, & \Theta_0 &= I, \\ \Theta_k D_{(k+1)l}(E, N) &= D_{(1)l}(E, N) - D_{(1)l}(E, k), \\ \Theta_k D_{(k+1)k+1}(E, N) &= D_{(1)k+1}(E, N), & 1 \leq l \leq k \leq N \leq \infty \end{aligned} \tag{11}$$

which may be verified by direct insertion into (7). The connection of the 'reduction' matrix Θ_k with the 'cut-off' sequence $F_j(E, k)$ has an important consequence: using the exact identity

$$\Theta_{k-1}|Y_k\rangle = \sum_{i=1}^j \Theta_{k-1}D_{(k)i}(E, j)|X_i\rangle + \Theta_j|Y_{j+1}\rangle, \quad j \geq k \geq 1 \tag{12}$$

and the iterative increase of the parameters k, j (convergence test), we may arrive at the reliable choice of the cut-off $N = j \gg k = 1, N < \infty$ in the practical application of expansion (6) of $|Y_1^i\rangle$.

Obviously, for $M_{k+1} = M_k$ and $\det B_k \neq 0, k \geq 1$, a 'non-reduced' form of (11), (12) may be given. Since the multiplication by B_k^{-1} enables us to calculate $D_{(k+1)j}, j \leq k$ directly from the second line in (7), it suffices to replace the third line in (11) by

$$B_k D_{(k+1)k+1} = \left((EI - A_k)D_{(k)k} - \sum_{i=1}^{k-1} C_{k(k-i)}D_{(i)k} \right) B_k F_{k+1}. \tag{11a}$$

Multiplication of (12) by Θ_{k-1}^{-1} provides

$$|Y_k\rangle = \sum_{i=1}^N D_{(k)i}(E, N)|X_i\rangle + D_{(k)N}(E, N)B_N|Y_{N+1}\rangle \tag{12a}$$

which represents a restoration of full analogy with I in this special case.

4. An application in nuclear theory

In Brueckner theory, the Bethe–Goldstone equation has the kernel

$$\mathfrak{Q} = \frac{\hat{q}}{\hat{q}(T + \omega)\hat{q}} \tag{13}$$

where T is kinetic energy, ω a parameter and \hat{q} the Pauli projector (Baranger 1969). One of the main technical problems of its exact solution is the evaluation of the matrix elements of \mathfrak{Q} in the double harmonic oscillator basis $|n_1 l_1\rangle |n_2 l_2\rangle$. Taking into account the action of the differential operator T and the definition of \hat{q} we simply put

$$|X_k^i\rangle \rightarrow \langle \kappa_1 \kappa_2 | X_k^i \rangle \rightarrow \langle \kappa_1 l_1 \kappa_2 l_2 | X_k^i \rangle = R_{n_1+i_1, l_1}(\kappa_1) R_{n_2+i_2, l_2}(\kappa_2),$$

$$i = n_1 + 1, k = n_2 + i_1 + 1,$$

$$\hat{q} = \sum_{k,i} |X_k^i\rangle \langle X_k^i|, \quad \hat{H} = -\hat{q}T\hat{q}, \quad T \sim \kappa_1^2 + \kappa_2^2, \quad E = \omega \tag{14}$$

where oscillator functions $R_{nl}(\kappa)$ of the impulse κ in the l th partial wave are defined in I. Different choices of $i_1 \geq 0, i_2 \geq 0$ lead to different Pauli projectors \hat{q} and correspond therefore to different nuclei (cf table 1: $F = 1$ for ^4He , $F = 2$ for ^{16}O and $F = 3$ for ^{40}Ca). The resulting matrix Q is quasitridiagonal ($C_{k(j)} = 0, j \geq 2$) and has growing partitions (e.g. $M_k = k$ for $i_1 = i_2 = 0$).

For matrix elements of \mathfrak{Q} needed in some M -dimensional space spanned by the orthogonal vectors $|X_k^i\rangle$, we redefine the partitioning of Q ($M'_1 = M_1 + M_2 + \dots + M_n > M, M'_{i+1} = M_{n+i}$) and pick up a sufficiently large cut-off N to obtain the desired accuracy. The high rate of convergence with respect to N and the low computer storage demands (= cca N^2 , to be compared with $\sim N^4$ for general matrix Q with dimension $M_1 + \dots + M_N$) are demonstrated in table 1 where the error of $\langle X_1^1 | \mathfrak{Q} | X_1^1 \rangle$ in the last column is comparable with the computer precision. This was

Table 1. Convergence of the lowest non-trivial matrix elements of the exact propagator \mathfrak{Q} with the cut-off N .

l_1	l_2	i_1	i_2	F	N		
					10	15	20
0	0	0	0	0	0.321 155	0.321 195	0.321 198
		1	1	1, 2	0.155 234	0.155 256	0.155 258
		2	2	3	0.102 423	0.102 440	0.102 441
1	0	0	0	0	0.247 661	0.247 679	0.247 680
		0	1	1	0.175 671	0.175 685	0.175 686
		1	1	2	0.136 281	0.136 296	0.136 297
2	0	0	0	0	0.200 455	0.200 463	0.200 464
		0	1	1	0.149 184	0.149 190	
		1	1	2	0.121 138	0.121 148	0.121 149
2	1	0	0	0, 1	0.167 922	0.167 926	0.167 926
		0	1	2	0.131 968	0.131 972	0.131 973
		1	1	3	0.108 756	0.108 762	0.108 762
2	2	1	1	3	0.098 565	0.098 569	0.098 569

independently tested by remultiplication by the original sparse matrix $\hat{q}(T + \omega)\hat{q}$. It should be noted that the numerically stable calculational procedure is very similar to that used in I for approximate \mathfrak{A} —we ‘scale’ the matrices $F_k \rightarrow \bar{F}_k = \rho_k F_k$ by the number $\rho_k \geq \rho_{0k} = i_1 + i_2 + k$ in recurrence relation (8).

5. Conclusions

There are two aims of the Born series parametric (polynomial) rearrangement:

- (a) simplification of the individual members of the expansion;
- (b) possible acceleration of convergence.

Both may be met using the present prescriptions together with:

- (a) the freedom to write $\hat{H}|X_k\rangle$ as a superposition of an arbitrary finite number of components $|X_{k+1}\rangle$, or
- (b) the knowledge of a sparse matrix representation of \hat{H} .

Thus, either

- (a) Q is varied to construct the simplest set $|X_k\rangle$, or
- (b) the orthonormalised basis is varied to obtain the special form of Q .

We summarise that in the case (a), the iterative formulae represent the direct generalisation of the standard identities

$$\begin{aligned} (E - \hat{H})^{-1} &= E^{-1} + E^{-1}\hat{H}(E - \hat{H})^{-1} \\ (E - \hat{H})^{-1} &= -\hat{H}^{-1} + \hat{H}^{-1}E(E - \hat{H})^{-1} \end{aligned} \tag{15}$$

corresponding in the case of the simplest Q (Haydock 1974) to the technique of § 3 and appendix 2, respectively. In the $\hat{q}T\hat{q}$ example presented, we have seen both the seminumerical structure (fixed analytic basis, calculated expansion coefficients) of the typical (a) approach application of non-trivial Q , and the pure numerical algorithm based on the (b) approach, very efficient (compared, for example, to the Gauss elimination) in the cases where we are interested in some submatrix of the whole resolvent matrix.

Appendix 1

When compared with the usual Born series, the domain of convergence of the present expansion (6) may be larger. We may illustrate this by an example with $M_k = M = 1$. Let us write

$$|X_j^1\rangle = |X_j\rangle = \sum_{\lambda} a_{\lambda(j)}|\lambda\rangle, \quad j \geq 1 \tag{A1}$$

where $|\lambda\rangle$ are eigenvectors of \hat{H} . The definition (2) may be shown to lead to

$$a_{\lambda(k)} = a_{\lambda(1)}(-1)^{k-1}\Delta_1^{(k-1)}(\lambda)/(B_1B_2 \dots B_{k-1}), \quad k \geq 2 \tag{A2}$$

where $\Delta_k^{(l)}(E)$ denotes determinant of the submatrix of $Q - E$,

$$\Delta_k^{(l)}(E) = \det \begin{pmatrix} Q_{kk} - E & Q_{kk+1} \dots & Q_{kl} \\ \vdots & & \\ Q_{lk} & \dots & Q_{ll} - E \end{pmatrix} \quad l \geq k. \tag{A3}$$

Since

$$\Delta_k^{(N)}(E) = (-1)^{N-k+1} / (F_k(E, N)F_{k+1}(E, N) \dots F_N(E, N)) \tag{A4}$$

the residual term in (12) is, for $k = 1$, equal to

$$D_{(1)N}(E, N)B_N|Y_{N+1}\rangle = \sum_{\lambda} \frac{a_{\lambda(1)}\Delta_1^{(N)}(\lambda)}{(E-\lambda)\Delta_1^{(N)}(E)}|\lambda\rangle \tag{A5}$$

and should approach zero for $N \rightarrow \infty$. This may be achieved either for diminishing ratio $\Delta_1^{(N)}(\lambda)/\Delta_1^{(N)}(E)$ (it works in Born series for $|\lambda/E| < 1$) or by demanding $\Delta_1^{(N)}(\lambda_i) \rightarrow 0, N \rightarrow \infty$ for 'inconvenient' λ_i 's (compare with the acceleration of convergence of the Born series by the special choice of vector $|X_1\rangle$ with $a_{\lambda_i(1)} = 0$). The limit $\Delta_1^{(\infty)}(\lambda) = 0$ may also be guaranteed for all λ 's by Q chosen as matrix elements of \hat{H} in an arbitrary basis.

Appendix 2

Definition (8) of the fundamental sequence $F_k(E)$ has the structure of the matrix continued fraction. Therefore, the inversion $(F_k^{-1})^{-1}$ must be well defined, $\det F_k^{-1} \neq 0, k \geq 1$. *Vice versa*, for $E = E_0$ such that there exists $k = i_0 > 1, \det F_{i_0}^{-1} = 0$, the sequence $F_k(E_0), k < i_0$ cannot be defined (some examples of such a 'pathological' behaviour may be found e.g. in Wilkinson 1965).

The first solution of this problem is based on the arbitrariness of M_k and consists in repartitioning of Q . This represents one of the significant advantages of the present method and needs no further comment.

In this appendix, we give another method, applicable when the partition redefinition is not desirable since $M_k = M$ is fixed. Then we may assume $\det B_k \neq 0$ and introduce formally the matrices $\Gamma_{k(i)}$ by the prescription

$$\Gamma_{k(-1)} = B_k, \quad \Gamma_{k(i)} = \Gamma_{k(i-1)}B_{k-i}^{-1}F_{k-i}^{-1}, \quad k > i. \tag{A6}$$

They have the properties

$$\Gamma_{k(i)} = F_k^{-1}B_{k-1}^{-1}F_{k-1}^{-1}B_{k-2}^{-1} \dots F_{k-i+1}^{-1}B_{k-i}^{-1}F_{k-i}^{-1}, \quad i \geq 0 \tag{A7}$$

$$\Gamma_{k(k-i)}^{-1}\Gamma_{k(k-j-1)}B_j^{-1} = F_iB_i \dots F_{j-1}B_{j-1}F_j, \quad 0 < i \leq j \tag{A8}$$

which follow easily from the definition. It is important that for $k = i_0, \det F_{i_0}^{-1} = 0$, the initialisation $\Gamma_{i_0(0)} = F_{i_0}^{-1}$ may be used to define the sequence

$$\dots F_{i_0+2}, F_{i_0+1}, \Gamma_{i_0(0)}, \Gamma_{i_0(1)}, \dots, \Gamma_{i_0(i_0-1)}$$

instead of F_k 's by using the following recurrence relation:

$$\Gamma_{k(k-m)} = -C_{k(k-m)} - \Gamma_{k(k-m-1)}B_m^{-1}(A_m - EI) - \sum_{i=1}^{k-m-1} \Gamma_{k(k-m-i-1)}B_{m+i}^{-1}C_{m+i(i)} - \sum_{i=1}^{\infty} (B_kF_{k+1} \dots B_{k+i-1}F_{k+i})C_{k+i(k+i-m)}, \quad m = k-1, k-2, \dots, 1 \tag{A9}$$

It is also easy to prove that the expansion coefficients in (6) may be redefined in terms of the new sequence

$$\{F_k\}_{k=i_0+1}^{\infty} \vee \{\Gamma_{i_0(k)}\}_{k=0}^{i_0-1}$$

e.g. in the case of (10), we obtain the relations

$$D_{(1)k}(E, N) = \Gamma_{i_0(i_0-1)}^{-1}(E, N) \bar{D}_k(E, N),$$

$$\bar{D}_k(E, N) = \begin{cases} \Gamma_{i_0(i_0-k-1)}(E, N) B_k^{-1}, & k \leq i_0, \\ B_{i_0} F_{i_0+1}(E, N) \dots B_{k-1} F_k(E, N), & k > i_0. \end{cases} \quad (A10)$$

The inversion of the $\Gamma_{i_0(i_0-1)}$ matrix necessarily exists for $\det(Q - E) \neq 0, N < \infty$, since the relation

$$\det(Q - E) = (-1)^{MN} \left(\prod_{i=1}^{i_0-1} \det B_i \right) \det \Gamma_{i_0(i_0-1)} \left(\prod_{i=i_0+1}^N \det F_i \right)^{-1}$$

follows directly from the decomposition (4) and (A7).

The occurrence of the singularity of the type $\det F_{i_0}^{-1} \rightarrow 0, E \rightarrow E_0$ is connected with the accidental zero of the subdeterminant of $Q - E$ for some values of the parameter $E = E_0$. Because of the continued fraction structure of the definition of F_k 's, usually a small repartitioning is sufficient—considering the simple one-dimensional example we see that only $(M_{i_0} = 1) \rightarrow (M_{i_0} = 2)$ is needed. The restoration of the F_k sequence may therefore be possible after a few 'intermediate' terms $\Gamma_{i_0(i_0-j)}, i_0 \leq j < i_1$ within the sequence F_k . Such a possibility occurs for some $i_1 > 1$ such that $\det \Gamma_{i_0(i_0-i_1)} \neq 0$. Then the identities

$$F_{i_1} = \Gamma_{i_0(i_0-i_1)}^{-1} \Gamma_{i_0(i_0-i_1-1)} B_{i_1}^{-1} \quad (A11)$$

$$F_{i_1} B_{i_1} F_{i_1+1} = \Gamma_{i_0(i_0-i_1)}^{-1} \Gamma_{i_0(i_0-i_1-2)} B_{i_1+1}^{-1}$$

etc may be inserted into definition (8) which generates $F_k, i_1 \geq k \geq 1$. In such a way, the restoration is completed.

Putting formally $i_0 = N, i_1 = 0$, the whole auxiliary sequence $\{\Gamma_{N(k)}\}_{k=0}^{k=N-1}$ may be used instead of $\{F_k\}_{k=N}^{k=1}$. Recurrence (A9) and formulae (A10) may represent the alternative version of our expansion of the resolvent operator while the iteration formula may read

$$B_N |Y_{N+1}\rangle = - \sum_{i=1}^N \Gamma_{N(N-i-1)}(E, N) B_i^{-1} |X_i\rangle + \Gamma_{N(N-1)}(E, N) |Y_1\rangle. \quad (A12)$$

At present, we do not encourage the use of this alternative scheme for 'physical' \hat{H} since our experience strongly supports the continued fraction approach. The Γ -generated 'polynomial' formulae do not seem to have a 'perturbative' character and should be more thoroughly investigated in the future.

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