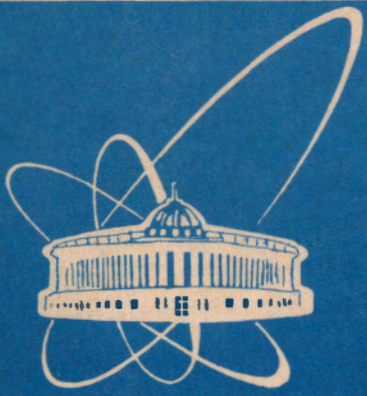

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THE COUPLED-CHANNEL *T*-MATRIX: ITS LOWEST-ORDER BORN + LANCZOS APPROXIMANTS

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Многоканальная T-матрица: её приближения по Борну + Ланцошу

Три итерационных метода решения уравнений типа Липпмана—Швингера (именно метод цепных дробей Горачека и Сасакавы [Phys.Rev., A28, 2151, 1983]), его модификация для борновских рядов с остатками [M.Znojil, Phys,Rev., A34, 2697, 1986] и многоканальное обобщение матрично непрерывных дробей [M.Znojil, Phys.Rev., A30, 2080, 1984] интерпретируются как специальные случаи общего итерационного матричного предписания. Во-первых, в терминах определенных асимметричных проекторов $P = P^+$ выводятся снова три старых частных метода как различные реализации хорошо известной инверсии Ланцоша. Затем предлагается обобщенный итерационный метод как перестройка борновского типа для произвольного итерационного шага по Ланцошу. Максимальная гибкость достигается в формализме, который может конкурировать со стандартным пересуммированием по Паде. Поэтому приводятся несколько первых приближений.

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Znojil M. E4-95-340

The Coupled-Channel T-Matrix:
Its Lowest-Order Born + Lanczos Approximants

Three iterative methods of solution of the Lippmann-Schwinger equations (viz., the method of continued fractions by J.Horáček and T.Sasakawa [Phys.Rev., A28, 2151 (1983)], its Born-remainder modification [M.Znojil, Phys.Rev., A34, 2697 (1986)] and a coupled-channel matrix-continued-fraction generalization [M.Znojil, Phys.Rev., A30, 2080 (1984)] are all interpreted as special cases of a common iterative matrix prescription. Firstly, in terms of certain asymmetric projectors $P \neq P^+$, we re-derive the three particular older methods as different realizations of the well-known Lanczos inversion. Then, a generalized iteration method is proposed as a Born-like re-arrangement of any intermediate Lanczos iteration step. A maximal flexibility is achieved in the formalism which might compete with the standard Padé re-summations in practice. Its first few truncations are listed, therefore.

The investigation has been performed at the Bogoliubov Laboratory of Theoretical Physics, JINR.

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1 Introduction

Scattering phenomena occupy a slightly exceptional position in quantum mechanics: They belong to the utterly basic experimental tools [1] while their theory keeps posing a number of conceptual challenges [2]. We intend to pay attention to some purely formal aspects of the underlying Lippmann-Schwinger-like equations

$$|\varphi\rangle = |u\rangle + GV|\varphi\rangle \tag{1}$$

and especially to the methods of their solution. We are going to describe certain climax of our lasting effort and apply here, in an explicit manner, several implicit ideas of C. Lanczos [3].

Lanczos' ideas proved useful in various areas of physics ranging from the nuclear structure or scattering studies and atomic and statistical physics up to elaborate calculations in the lattice gauge field theory [4]. Certain unclarified formal aspects made some of their older applications related to the atomic, molecular and/or nuclear scattering [5, 6] less understood from the purely mathematical point of view. Especially, a dissatisfaction may concern the coupled-channel constructions of the Born-series remainders. Up to now, they remain incomplete and unsatisfactory [7]. In this paper, we are going to fill the gap and to clarify and resolve a few pertaining puzzles.

We may start by reminding the reader that measurable characteristics of scattering (e.g., phase shifts) may be calculated via the Lippmann-Schwinger-like equation (1) from the overlaps $\langle u|V|\varphi\rangle$ where V denotes the interaction operator and G (or, more conventionally, G_0) is a V-independent free Green's function. The "ket" symbol $|u\rangle$ represents the incoming wave [1]. For the scattering which goes through N channels,

$$\langle r|u\rangle = (\langle r|u\rangle_1, \langle r|u\rangle_2, \ldots, \langle r|u\rangle_N) \tag{2}$$

with an N-plet of the eligible incident waves $\langle r|u\rangle_j$ [functions of (a set of) coordinates $r = \{r_1, \ell_1, \ldots\}$] numbered by some (multi-) index $j = 1, 2, \ldots N$, we shall assume that one wishes to compute the whole set of the N^2 elements $\langle u|V|\varphi\rangle \equiv \langle u|T|u\rangle$ of the so called T-matrix at once [8].

In numerical context, iterations of the Lippmann-Schwinger-type equation (1) and the common n-th Born approximation

$$\langle u|V|\varphi\rangle = \langle u|V|u\rangle + \langle u|VGV|u\rangle + \ldots + \langle u|V\underbrace{(GV)(GV)\ldots(GV)}_{(n-1)-\text{times}}|u\rangle + R \quad (3)$$

with $R \approx 0$ serve the purpose as one of the most frequent methods. Once it fails, an alternative solution to equations (1) may be based on their algebraic re-interpretation and direct inversion,

$$\langle u|T|u\rangle \equiv \langle u|V\frac{1}{1-GV}|u\rangle. \quad (4)$$

At $N = 1$, one of the most elegant and appealing realizations of the latter scheme is due to Horáček and Sasakawa [9]. Their approach (called the method of continued fractions) is based on an iterative separable expansion of the interactions V. In ref. [6], it was shown that the resulting prescription is mathematically equivalent to the Lanczos algorithm [10].

For purposes of global analysis of the complicated coupled-channel scattering, an adaptation and $N > 1$ generalization of the original method of Horáček and Sasakawa has been described in our 1984 comment [5]. The new formalism offered the analogous, matrix continued fraction formulas for the $N \times N$ dimensional matrices of observables $\langle u|T|u\rangle$, technically facilitated by an appropriate extension (namely, by a partitioned-matrix modification, cf. [11]) of the underlying Lanczos prescription.

The rate of convergence of the Born as well as Lanczos iterations depends on the (*a priori*, unknown) subtle properties of G, V and $|u\rangle$ [1]. This inspired our empirical study [6] of a combined method: In the pre-iterated Lippmann-Schwinger equation (3), only the remainder R was represented as a Horáček-Sasakawa-like continued fraction. Numerical tests of the latter strategy proved

encouraging but their numerical scope as well as detailed description was basically restricted to the uncoupled channels only, $N = 1$. Here, we shall contemplate all finite integers $N \geq 1$. In a perspective close to the language of Löwdin [12] and Feshbach [13], we shall introduce certain suitable sequences of projection operators and re-derive the older prescriptions anew. We intend to profit from the related new interpretation of the Lanczos "vertical-iteration" prescriptions (Sect. 2). In particular, we notice that in each step of the vertical iterations, a Born-like (= "horizontal") improvement of the remainder term becomes very easy in the new language. In Sect. 3, we develop this idea in more detail and arrive at the whole new hierarchy of approximants which mix the horizontal and vertical iterations into a (virtually arbitrary) blend. Many adjacent methodical questions will be left aside. Recalling the numerical tests of ref. [6] as an implicit support of our expectations, we shall even avoid any additional numerical illustration. Its role could be quite supportive in general, but we consider the credit of simple examples undeservedly high in the community: One may almost always pre-determine the success of unrealistic illustrations by their sufficiently sophisticated (or sufficiently patient trial-and-error) choice. At the same time, we did not pursue any particular application. Thus, our paper remains short and Section 4 already becomes its summary.

2 Iterations

In what follows, abbreviation

$$R = \langle 0^*|\frac{1}{1-GV}|0\rangle, \quad \langle 0^*| \equiv \langle u|V(GV)^s, \quad |0\rangle \equiv (GV)^t|u\rangle \quad (5)$$

may and will denote both the desired measurable submatrix $\langle u|T|u\rangle$ of the T-matrix (at $s = t = 0$) and its remainder in eq. (3) (whenever $s + t = n - 1 > 0$). In this notation, let us re-derive the older continued fraction (CF) methods in their new, Löwdin-Feshbach-like re-interpretation, based on an introduction of a suitable pair of projectors $P = P^2$ and $Q = 1 - P$.

2.1 Projections

With the requirement of validity of the properties $P|0\rangle = |0\rangle$ and $\langle 0^*|P = \langle 0^*|$, let us define $P = P_0$ by the formula

$$P_0 = |0\rangle \frac{1}{\langle 0^*|0\rangle} \langle 0^*|. \tag{6}$$

Such a definition is asymmetric, i.e., $P \neq P^+$ and $Q = Q_0 \neq Q^+$. In the literature, this is a rather unusual choice – for many reasons one often prefers symmetric constructions, in spite of a necessity of using the square roots of operators [14]. In ref. [6], it was precisely such a requirement of symmetry which made our basis incompletely orthogonalized. Later on, we shall see that our present choice of asymmetric projectors offers the most natural and long-sought solution of this non-orthogonality problem.

In the first step, we may write, in a little bit formal way,

$$R = \langle 0^*| \frac{1}{1 - GV} |0\rangle = \langle 0^*| P \frac{1}{1 - GV} P |0\rangle \tag{7}$$

and try to interpret this T-submatrix (or just its Born remainder in general) as a result of inversion of the operator $1 - GV$ in a $(P + Q)$-partitioned space. In linear algebra the partitioned inversion proceeds in accord with the

formula

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-1} = \begin{pmatrix} (A - BD^{-1}C)^{-1} & \dots \\ \dots & \dots \end{pmatrix} \tag{8}$$

where A, B, C and D are arbitrary submatrices and D is assumed nonsingular. The explicit use of projectors P and Q implies the parallel operator identity

$$P \frac{1}{\mathcal{M}} P = P \frac{1}{P\left(\mathcal{M} - \mathcal{M} Q \frac{1}{Q\mathcal{M}Q} Q\mathcal{M}\right) P} P. \tag{9}$$

With the choice of $\mathcal{M} = 1 - GV$, the left-hand-side of the identity coincides with our key quantity $R = R_0$,

$$R_0 = \langle 0^*|0\rangle \frac{1}{\langle 0^*|(1 - GV)|0\rangle - R_1} \langle 0^*|0\rangle. \tag{10}$$

On the right-hand side, we abbreviated

$$R_1 = \langle 1^*| Q \frac{1}{Q(1 - GV)Q} Q |1\rangle, \quad |1\rangle = QGV|0\rangle, \quad \langle 1^*| = \langle 0^*|GVQ \tag{11}$$

and guaranteed the bi-orthogonality

$$\langle 0^*|1\rangle = 0, \quad \langle 1^*|0\rangle = 0 \tag{12}$$

which is due to the presence of the projectors $Q = Q_0$.

2.2 Vertical iterations

We may notice that formula (10) re-expresses the original full-space inversion of $\mathcal{M} = 1 - GV$ in terms of an inversion of the same operator in a subspace. Moreover, once we introduce an auxiliary symbol $Q_{-1} \equiv 1$ and write

$$R_0 = \langle 0^*|Q_{-1}\frac{1}{Q_{-1}(1-GV)Q_{-1}}Q_{-1}|0\rangle \tag{13}$$

we see that the observable R_0 and remainder R_1 have precisely the same form. We may say that equation (10) eliminates the zeroth Lanczos vectors $\langle 0^*|$ and $|0\rangle$ from our scope completely. With the "next", bi-orthogonal pair of the Lanczos vectors $\langle 1^*|$ and $|1\rangle$, our task (namely, the full-space inversion and evaluation of the "in-the-model-space" quantity R_0) becomes reduced to the mere "out-of-the-model-space" inversion of a submatrix. Obviously, the whole elimination $Q_{-1} \to Q_0$ of the N-dimensional subspaces spanned by the respective bras $\langle 0^*|$ and kets $|0\rangle$ may be iterated.

In a purely numerical language and with $N = 1$, iterations of this type lead to the standard method of inversion of a finite matrix $p \times p$ with $R_{p+1} = 0$. In the limit $p \to \infty$, the infinite continued fraction formulas are produced [15]. They become a vertical parallel or counterpart to the standard horizontal infinite Born series. In the present $N > 1$ setting related to ref. [5], the

explicit derivation of the matrix CF formulas remains the same. Firstly, projectors

$$P_k = |k\rangle\frac{1}{\langle k^*|k\rangle}\langle k^*|, \quad Q_k = Q_{k-1} - P_k \tag{14}$$

and recurrences

$$|k+1\rangle = Q_k GV|k\rangle, \quad \langle (k+1)^*| = \langle k^*|GVQ_k, \quad k = 1, 2, \ldots \tag{15}$$

define the next (N-plets of) Lanczos basis vectors. In contrast to the parallel but unfinished construction of ref. [6], they stay bi-orthogonalized. In a similar vain, residual quantities (matrices)

$$R_{k+1} = \langle (k+1)^*|Q_k\frac{1}{Q_k(1-GV)Q_k}Q_k|k+1\rangle, \qquad k = 0, 1, \ldots \tag{16}$$

obey the same recurrent CF (i.e., matrix-CF) rule

$$R_k = \langle k^*|k\rangle\frac{1}{\langle k^*|k\rangle - \langle k^*|GV|k\rangle - R_{k+1}}\langle k^*|k\rangle. \tag{17}$$

Now, in order to arrive at the standard definition of the infinite CF expansion, it is sufficient to choose the initial $R_{K+1} = 0$ in the limit $K \to \infty$. We may summarize: For all $N > 1$, the iterative representation of T-matices is now well understood. The underlying matrix CF expansions may rely on the recent progress in mathematics [16]. In our notation with $s \geq 0$ and $t \geq 0$ in

eq. (5), the special "horizontal-followed-by-vertical" $s+t>0$ formalism of ref. [6] extends its applicability to the $N>1$ coupled channels immediately.

2.3 Vertical and horizontal iterations mixed

For practical purposes, an important byproduct of our clear separation of the horizontal and vertical iterations lies in the obvious possibility of their combinations. Within this program, it seems desirable to find a list and/or classification of all (or rather, from the purely pragmatic point of view, of the first few) combined Born + CF approximants. In the summary of the $N=1$ numerical tests in ref. [6], we also emphasized certain complementary character of the vertical ($Q_k \to Q_{k+1}$) and horizontal (Born) iterations. Generically, the vertical improvements of precision varied with the particular characteristics of V. Numerically, they seemed less energy-dependent. At the same time, the horizontal convergence is well known to improve with the growing energies significantly. The latter empirical experience is to be understood as a guide to the general formation of approximants which would go beyond the simple once-iterated level. Whenever we spot an inefficiency of a horizontal step, we may feel obliged to try its vertical counterpart, and *vice*

versa. In a more detailed discussion, for the sake of clarity, let us mark, whenever needed, each horizontal or vertical iteration step by a (superscripted) horizontal or vertical arrow "$\rightarrow$" or "$\Downarrow$", respectively. With this convention, the unique, exceptional and virtually trivial first Born approximation

$$\langle u|T|u\rangle^{(\rightarrow)} = \langle u|V|u\rangle \tag{18}$$

is the only prescription which does not contain any factor G at all. The first nontrivial parallel realization of the downwards CF scheme (namely, the one with the vanishing R_1) gives

$$\langle u|T|u\rangle^{(\Downarrow)} = \langle u|V|u\rangle \frac{1}{\langle u|V|u\rangle - \langle u|VGV|u\rangle} \langle u|V|u\rangle. \tag{19}$$

It already contains a factor G, i.e., virtually, the same amount of information and/or computational effort as required by its second-order Born alternative

$$\langle u|T|u\rangle^{(\rightarrow\rightarrow)} = \langle u|V|u\rangle + \langle u|VGV|u\rangle. \tag{20}$$

This explains the doubling of the vertical arrows in our notation. The multiplicity N_G of the occurrence of G's in each inner product characterizes, in a very rough estimate, the computer time needed for its evaluation via numerical integrations and/or summations. Hence, computational complexity of all

the higher-order approximants may and, tentatively, will be characterized by the magnitude of the maximal N_G.

3 Truncations

For the slowly convergent (sometimes even divergent) infinite Born expansions (3) ($N_G \to \infty$), one may often find their correct sum by means of their so called Padé resummation [17]. Continued fractions are then recalled as just one of many particular realizations of numerical acceleration of the horizontal convergence. In the present context, the formal source of the alternative, vertical CF iterations is entirely different and much deeper (e.g., V-dependent – cf. the preceding section). As a consequence, a large uncertainty in the remainder R_1 is believed to lead to a reasonable and acceptable precision of the computed T-matrix elements R_0. The "over-optimistic" convergence assumptions of this type emerge in the closely interrelated "effective-Hamiltonian" constructions by Löwdin [12] as well as in their "doorway-hallway" parallels by Feshbach et al [13].

In complicated systems, similar optimism and drastic $N_G \ll \infty$ approximations (complemented or supported also, e.g., by variational considerations

[18]) may form the only feasible computation recipe. Its succes and failures crucially depend on the operators in question. In the less favourable cases, universal recipes do not exist. Hence, various partial solutions of this methodical problem are permanently called for. A partial answer to the challenge is to be offered here as well. Basically, in a way completing our preceding papers, we shall search for a suitable combination of the horizontal and vertical iterations, and propose to blend them in arbitrary $N_G \ll \infty$ sequences and combinations. The older pure-Born and pure-Lanczos approximations reflect and represent just the two extreme possiblilities.

3.1 Approximations with $N_G = 2$

After we perform the necessary input overlap integrations involving the singlets and pairs of G's, we encounter the three possible approximative definitions of the observables R_0 ($s = t = 0$). The first one coincides with the third-order Born sum

$$\langle u|T|u\rangle^{(\rightarrow\rightarrow\rightarrow)} = \langle u|V|u\rangle + \langle u|VGV|u\rangle + \langle u|VGVGV|u\rangle. \qquad (21)$$

The next one enriches the simplest CF denominator by the first-order Born remainder added,

$$\langle u|T|u\rangle^{(\Downarrow\rightarrow)} = \langle u|V|u\rangle \frac{1}{\langle u|V|u\rangle - \langle u|VGV|u\rangle - \langle v^*|v\rangle} \langle u|V|u\rangle. \qquad (22)$$

We see that the approximant already involves the higher Lanczos projected basis states in an overlap,

$$\langle v^*|v\rangle = \langle u|VGVGV|u\rangle - \langle u|VGV|u\rangle (\langle u|V|u\rangle)^{-1} \langle u|VGV|u\rangle. \qquad (23)$$

Finally, the third arrangement

$$\langle u|T|u\rangle^{(\rightarrow\Downarrow)} = \langle u|V|u\rangle + \langle u|VGV|u\rangle \frac{1}{\langle u|VGV|u\rangle - \langle u|VGVGV|u\rangle} \langle u|VGV|u\rangle \qquad (24)$$

is easily interpreted as the first nontrivial combination of Born series with a CF estimate of its remainder.

3.2 Approximations with $N_G = 3$

With an insufficiently rapid convergence, physical predictions of the four-term Born approximants $\langle u|T|u\rangle^{(\rightarrow\rightarrow\rightarrow)}$ may be improved by a universal Padé resummation [17]. In the present context with triplets of G's in the related overlap evaluation, better chances of preservation of computational

investments [19] might still be assigned to the twice iterated CF prescription $\langle u|T|u\rangle^{(\Downarrow\Downarrow)}$, i.e.,

$$\langle u|V|u\rangle \frac{1}{\langle u|V|u\rangle - \langle u|VGV|u\rangle - \langle v^*|v\rangle \frac{1}{\langle v^*|v\rangle - \langle v^*|GV|v\rangle} \langle v^*|v\rangle} \langle u|V|u\rangle \qquad (25)$$

or to the alternative formula

$$\langle u|T|u\rangle^{(\Downarrow\rightarrow)} = \langle u|V|u\rangle \frac{1}{\langle u|V|u\rangle - \langle u|VGV|u\rangle - \langle v^*|v\rangle - \langle v^*|GV|v\rangle} \langle u|V|u\rangle \qquad (26)$$

where, within the Q-projected subspace, the remainder R_2 has been expanded in the second-order Born way. In the present scheme, the next prescription, namely, $\langle u|T|u\rangle^{(\rightarrow\Downarrow\rightarrow)}$ is, by its structure, a different formula

$$\langle u|V|u\rangle + \langle u|VGV|u\rangle \frac{1}{\langle u|VGV|u\rangle - \langle u|VGVGV|u\rangle - \langle w^*|w\rangle} \langle u|VGV|u\rangle \qquad (27)$$

with a nice exemplification of the less trivial "next" Lanczos vectors, say,

$$|w\rangle = GV|u\rangle - |u\rangle \frac{1}{\langle u|VGV|u\rangle} \langle u|VGVGV|u\rangle \qquad (28)$$

and

$$\langle w^*| = \langle u|VGVGV - \langle u|VGVGV|u\rangle \frac{1}{\langle u|VGV|u\rangle} \langle u|VGV. \qquad (29)$$

It "regularly" alternates the CF and Born steps in a way which reminds us of one of the well known equivalence transformations of the ordinary (scalar)

analytic continued fractions [20]. Finally, a return to simplicity seems characteristic for the remainder

$$\langle u|VGVGV|u\rangle \frac{1}{\langle u|VGVGV|u\rangle - \langle u|VGVGVGV|u\rangle} \langle u|VGVGV|u\rangle \quad (30)$$

(i.e., difference $\langle u|T|u\rangle^{(\rightarrow\rightarrow\rightarrow)} - \langle u|V|u\rangle - \langle u|VGV|u\rangle$) in the last, fifth $N_G = 3$ prescription.

3.3 Approximations with $N_G > 3$

The general pattern of forming the further and further re-arrangements of the standard Born series becomes clear. At the higher N_G's we get more and more approximants $\langle u|T|u\rangle^{(\clubsuit)}$ to our observables which blend the horizontal and vertical iterations together in all the possible ways. The total number $N_{(\clubsuit)}$ of these possibilities is equal to the (N_G+2)-nd Fibonacci number [21]. A sample of the first few eligible iteration patterns $\clubsuit$ (which could prove useful in applications) is enclosed here in Table 1.

For the sufficiently complicated systems, higher-order Born series are rarely used. Indeed, the necesssary numerical evaluation of the overlaps becomes already much more time-consuming than a purely numerical inversion of the operator $1 - GV$ itself, say, on a mesh of grid points [22]. Similarly,

the higher-order vertical iterations become less easy. More attention must be paid to non-commutativity of their "input", $N \times N$-dimensional overlap matrices in the $N > 1$ coupled-channel formulas and still, the overall complexity of the formulas grows quickly with the growing N_G. In many a respect [23], the choice of $N_G > 3$ remains restricted to the less complicated systems and/or to the explicit analysis of errors and/or perturbations.

3.3.1 Matrix moments

At $N_G > 3$, the notation must necessarily be made less cumbersome. Firstly, without any difficulty, we may further reduce the full bra and ket symbols "$\langle u|$" and "$|u\rangle$" to mere "$\langle$" and "$\rangle$", respectively. Secondly, we may notice that the interaction operators V always occur just between a pair of G's or between a G and an external bra or ket symbol. This means that the letter V plays a highly formal role of a "multiplication metric" [24]. Its use does not carry any information and the redundant V's need not appear in the formulas at all. Finally, being left with the sole G's between "$\langle$" and "$\rangle$", the only relevant information is just their number and we may put $\langle GGG\rangle = \langle 3\rangle$ etc. In this notation (reminding us of the use of moments in the $N = 1$ case

[25]), the overlap in eq. (27) acquires the compact form

$$\langle w^*|w\rangle = \langle 3\rangle - \langle 2\rangle \frac{1}{\langle 1\rangle} \langle 2\rangle \qquad (31)$$

etc. At the same time, new symbols must be invented for the higher-order Lanczos basis states (this will not be done here).

3.3.2 Perturbations

In the light of our horizontal-followed-by-vertical prescription of ref. [6] in its present non-commutative coupled-channel extension and denotation $\clubsuit^{(hv)} = (\rightarrow\rightarrow \ldots \rightarrow\Downarrow\Downarrow \ldots \Downarrow)$ it is interesting to return to the perturbative aspects of the Born series and compare, in this context, different perturbed as well as unperturbed prescriptions with each other. Thus, the $N_G = 3$ Born+remainder formula (30) with $\clubsuit^{(hv)} = (\rightarrow\rightarrow\Downarrow)$ repesents, for the sufficiently small kernels GV at least, a quasi-perturbative improvement of its (for the present purposes, slightly re-arranged) Born+CF $N_G = 2$ antecedant (24),

$$\langle u|T|u\rangle^{(\rightarrow\Downarrow)} - \langle 0\rangle - \langle 1\rangle = \langle 1\rangle \frac{1}{\langle 1\rangle - \langle 2\rangle} \langle 2\rangle \qquad (32)$$

or even of the $N_G = 1$ purely CF formula (19) in the parallel re-arrangement

$$\langle u|T|u\rangle^{(\Downarrow)} - \langle 0\rangle - \langle 1\rangle = \langle 1\rangle \frac{1}{\langle 0\rangle - \langle 1\rangle} \langle 1\rangle \qquad (33)$$

For practical purposes, similar comparisons of remainders might help as a support of reliability of results of all our less usual prescriptions.

A requirement of compatibility of all the available fixed-N_G approximants may prove more and more useful at the higher N_G's, where their number grows quickly. Another use of the alternative higher-order formulas may be connected with the possible (e.g., physical, perturbatively induced) variations of the interaction V or, alternatively, with some numerical uncertainties in the overlaps (error bars, an unprecise specification of, or a change of energy in, the propagator G, etc). Indeed, once we describe all these variations as a perturbation-like modification of the overlaps themselves,

$$\langle k^{(perturbed)}\rangle = \langle k^{(unperturbed)}\rangle + \lambda\langle k^{(correction)}\rangle + \lambda^2\langle k^{(next\ correction)}\rangle + \ldots, \qquad (34)$$

we may easily re-write the latter Born like re-arrangements of our formulas as power series in the (presumably, very small) parameter λ. This is a task which is not too complicated (cf. [26]) but takes us already too far beyond the scope of the present paper.

4 Summary

Old subject of solving the Lippmann-Schwinger equations was studied and re-interpreted as tractable via a generalized Lanczos algorithm in a partitioned biorthogonal basis. In a way which combines the standard Born-like horizontal iterations with the vertical Feshbach-like repeated projections, a formalism was obtained which replaces the standard Padé resummation by a more flexible and fully interaction-adapted algorithm. With the first few resulting matrix-Padé-like approximants being listed explicitly, the new inversion-iteration algorithm is equally well applicable to both the uncoupled and coupled-channel Lippmann-Schwinger equations.

The main idea of the prescription lies in our freedom of interchanging, at any stage of development of the approximant, the standard horizontal iterations (of the set of integral equations of the type (1)) with the non-standard vertical iterative projections of these equations on the suitable (we might call them Hilbert-Lanczos) subspaces. In this sense both the standard re-summations of the power series (say, by means of the fractional approximants) and the "purely vertical" Lanczos method find their common generalization. Due to its flexibility achieved by our re-arrangements, the

underlying matrix CF approximants already lie quite close to the general Padé approximants. Still, they do not share the unnecessarily complicated character of the latter concept (cf., e.g., [17], p. 270).

As a maximally natural technique of re-summation of the standard Born series, our present proposal, the long awaited completion of our older paper [6], offers an alternative to the universal Padé strategy. This point of view opens many new questions. The key one, asking for quantitative illustrations and applications, would necessarily be expensive to answer. In an immediate future, practical use of our formulas may be expected to emerge in analyses of a genuine coupled channel scattering, in particular as a new possibility of extraction of a complete set of observables from the tedious numerical input work, namely, from the time-consuming evaluation of overlap integrals.

On a methodical level, we may re-emphasize that our prescription results from a mixture of the Born-like and Lanczos-like points of view. Technically, it is sufficiently transparent. In the language of the matrix moments, the explicit (cf., e.g., eq. (33)) or implicit (e.g., eq. (32)) symmetry of our formulas follows from their independence of our detailed choice of the projectors, with the various possible splits of GV's between the vectors $\langle 0^*|$ and $|0\rangle$. Unfortunately, one may only hardly believe in a feasibility of any rigorous analyses of

convergence. As an empirical hint, we proposed the use of re-arrangements. It is only a very partial answer – the general and highly challenging problem of determination of some suitable external (e.g., variational or perturbative) "effective" initial quantities $R^{eff}_{K+1} \neq 0$ remains open.

Table 1. The complete list of re-arrangements $R_0^{(\clubsuit)}$ of the first few simplest Born approximants.

the order of approximation N_G+1	$\clubsuit$				
1	$\rightarrow$				
2	$\rightarrow\rightarrow$	$\Downarrow$			
3	$\rightarrow\rightarrow\rightarrow$	$\rightarrow\Downarrow$	$\Downarrow\rightarrow$		
4	$\rightarrow\rightarrow\rightarrow\rightarrow$	$\rightarrow\rightarrow\Downarrow$	$\rightarrow\Downarrow\rightarrow$	$\Downarrow\rightarrow\rightarrow$	$\Downarrow\Downarrow$
5	$\rightarrow\rightarrow\rightarrow\rightarrow\rightarrow$	$\rightarrow\rightarrow\rightarrow\Downarrow$	$\rightarrow\rightarrow\Downarrow\rightarrow$	$\rightarrow\Downarrow\rightarrow\rightarrow$	$\Downarrow\rightarrow\rightarrow\rightarrow$
	$\rightarrow\Downarrow\Downarrow$	$\Downarrow\rightarrow\Downarrow$	$\Downarrow\Downarrow\rightarrow$		
6	$\rightarrow\rightarrow\rightarrow\rightarrow\rightarrow\rightarrow$	$\rightarrow\rightarrow\rightarrow\rightarrow\Downarrow$	$\rightarrow\rightarrow\rightarrow\Downarrow\rightarrow$	$\rightarrow\rightarrow\Downarrow\rightarrow\rightarrow$	$\rightarrow\Downarrow\rightarrow\rightarrow\rightarrow$
	$\Downarrow\rightarrow\rightarrow\rightarrow\rightarrow$	$\rightarrow\rightarrow\Downarrow\Downarrow$	$\rightarrow\Downarrow\rightarrow\Downarrow$	$\Downarrow\rightarrow\rightarrow\Downarrow$	$\rightarrow\Downarrow\Downarrow\rightarrow$
	$\Downarrow\rightarrow\Downarrow\rightarrow$	$\Downarrow\Downarrow\rightarrow\rightarrow$	$\Downarrow\Downarrow\Downarrow\Downarrow$		

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[7] For example, we have succeeded in finding just a partially orthogonalized Lanczos-like basis set in the preceding reference.

[8] We shall drop the channel subscripts in what follows. Thus, the symbol (A) will always denote an $N \times N$-dimensional matrix, although its scalar interpretation at $N = 1$ is also admissible.

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[22] cf., e.g., the reivew of methods in C. Cerjan (ed.), Numerical Grid Methods and Their Application to Schrödinger's equation (Kluwer, Dordrecht, 1993).

[23] I.e., in a way parallelling the applications of the standard Padé approximants.

[24] The absence of normalizability of our incident-wave bras and kets ($\langle u|u\rangle = \infty$ for plane waves) would be a serious drawback without having the metric V and, by assumption, finite overlaps $\langle u|V|u\rangle < \infty$ etc. Mainly this idea would form a "missing link" between $N = 1$ and $N > 1$ in ref. [6].

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