# Phys. Lett. A - to appear:<br>The most general iteration scheme for the Lippmann-Schwinger-type equations

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## Abstract

$T$-matrix elements (i.e., phase shifts, etc.) are usually evaluated, iteratively, in their pure summation (Born – von Neumann) or pure fractional (Lanczos) representation. We propose a new and more flexible mixed scheme (one encounters the $(N+1)$-st Fibonacci number of alternatives in the $N$-th approximation) and discuss its properties.

# 1 Introduction and motivation

In the textbook quantum mechanics, Lippmann-Schwinger equation

$$|\varphi\rangle = |u\rangle + G_0 V|\varphi\rangle \tag{1}$$

defines the $T$-matrix elements $\langle u|V|\varphi\rangle \equiv \langle u|T|u\rangle$ pertaining to an interaction $V$ and to a $V$-independent Green's function $G_0$. In the simplest systems where "kets" $|u\rangle$ represent just plane waves, quantity $\langle u|T|u\rangle$ defines phase shifts. Even then, the description of scattering via eq. (1) remains non-trivial: The common iterative solutions

$$\langle u|T|u\rangle \approx \langle u|V|u\rangle + \langle u|VG_0V|u\rangle + \ldots + \langle u|V\underbrace{(G_0V)(G_0V)\ldots(G_0V)}_{(n-1)-\text{times}}|u\rangle \tag{2}$$

(viz., the $n$-th Born approximants) need not converge and necessitate a certain "sufficient smallness" of $K$ [1]. This motivated a deeper study of alternative techniques.

A significant progress has been achieved via a direct use of the operator inversion,

$$\langle u|T|u\rangle \equiv \langle u|V\frac{1}{1-G_0V}|u\rangle \tag{3}$$

able to deal with the "not too small" $K$'s. The more complicated character of the inversion proved at least partially compensated by a broad flexibility of the corresponding purely numerical approximation schemes. Within the framework of the particular Lanczos approach [2, 3]), one may even return to the quasi-analytic recurrent recipes. In the context of scattering theory, they were re-introduced as the so called method of continued fractions by Horáček and Sasakawa [4].

The numerical success of the continued fraction (CF) iterations was underlined by the subsequent observation [5] that the absence of normalizability of the standard incident plane-wave bras and kets, $\langle u|u\rangle = \infty$ does not spoil the CF recipe – one always encounters just the finite overlaps (e.g., $\langle u|V|u\rangle < \infty$)

in the formulae. At the same time, with the growing precision, their complexity proved to increase much more quickly than in the less sophisticated Born series (2).

It is well known that mathematically, the competition between prescriptions (3) and (2) is closely related to the (*a priori*, unknown) spectral properties of the kernel $G_0V$. In the majority of applications, one must proceed "experimentally", making a choice between prescriptions (3) and (2) in a trial-and-error manner. Here, we support and even extend such a pragmatic point of view. Indeed, the choice between eq. (3) and (2) is not the only possibility. We intend to list all the other, alternative iterative candidates for construction of approximants, therefore.

A core of our short note will lie in the introduction of a notation which will clarify mutual relations between the seemingly different older techniques. As a consequence, we shall be able to make a step beyond the existing recommendations [2]-[6] and propose a certain universal blend of the above-mentioned Born and Lanczos iterations.

We believe that the resulting possibility of simultaneous evaluation of many alternative "equivalent" approximants offers such a universal and flexible strategy of efficient approximate constructions of $\langle u|T|u\rangle$'s which might suit better the phenomenological purposes.

# 2 $T$-matrix and the standard iterations

In simplified models, the non-Hermitean kernel operator $G_0V \equiv K \neq K^+$ may be represented in a formally diagonalized form

$$K \equiv G_0V = \sum_j |f_j\rangle \varepsilon_j \langle g_j| \tag{4}$$

with $|f_j\rangle \neq |g_j\rangle$ in general. In this language, the divergence (as well as the rate of convergence) of the Born – von Neumann series (2) is simply controlled by the magnitude of eigenvalues $\varepsilon_j$, and the above-mentioned "sufficient smallness" of

$G_0V$ means, simply, $|\varepsilon_j| < 1$ for all $j$. The requirement is easily met in the high-energy regime (cf. [1]). The other Lanczos-inspired iteration schemes (cf also ref. [7] for their broader sample) are more difficult to analyse. In the forthcoming short review of two of them, we shall need a slightly more sophisticated notation, therefore.

## 2.1 The Horáček's and Sasakawa's continued fractions

Various versions of the direct inversion (3) may deal, satisfactorily, with the larger $\varepsilon_j$'s of eq. (4). The Lanczos algorithm proved particularly succesful in practice – the deeper reason might be traced to its shift of emphasis from eigenvalues to an optimal choice (or rather constructive selection) of the eigenvectors $|f_j\rangle$ and $\langle g_j|$. The older nuclear-physics study [8] might be recalled for a particularly impressive explicit illustration.

In the CF prescription of ref. [4], the Lanczos-type basis $|f_j\rangle$ and $\langle g_j|$ may be interpreted as born out of a systematic projective reduction of the interaction $V$ (cf. [5]). A specific feature of such an approach lies in its transparency, stemming from a consequent use of the concept of bi-orthogonality [9] which, basically, relaxes the demand of Hermitean conjugacy of the bra and ket basis states.

Let us mark the "second" basis by a $^\star$-superscript and, in a preliminary step, define $\langle u|V \equiv \langle 0^\star|$ and $|0\rangle \equiv |u\rangle \neq |0^\star\rangle \equiv V^+|u\rangle$. As long as our pair of these initial vectors need not be (bi-)normalized to one, we only assume that $0 \neq \langle 0^\star(s)|0(t)\rangle < \infty$ and introduce an operator

$$P = P_0 = |0\rangle \frac{1}{\langle 0^\star|0\rangle} \langle 0^\star|.$$

This is a non-Hermitean projector, $P^+ \neq P \equiv P^2$.

As long as $P|0\rangle = |0\rangle$ and $\langle 0^\star|P = \langle 0^\star|$, we may recall eq. (3),

$$\langle u|T|u\rangle = \langle 0^\star|\frac{1}{1-K}|0\rangle = \langle 0^\star|P\frac{1}{1-K}P|0\rangle$$

and re-write it via a partitioned ($P+Q=1$) operator identity

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

With $\mathcal{M}=1-K$, this gives the new formula for our $T$-matrix element,

$$\langle u|T|u\rangle \equiv R_0 = \langle 0^\star|0\rangle \frac{1}{\langle 0^\star|(1-K)|0\rangle - R_1}\langle 0^\star|0\rangle \tag{5}$$

where we abbreviated

$$R_1 = \langle 1^\star|Q\frac{1}{Q(1-K)Q}Q|1\rangle, \qquad |1\rangle = QK|0\rangle, \quad \langle 1^\star| = \langle 0^\star|KQ. \tag{6}$$

As a byproduct, the bi-orthogonality $\langle 0^\star|1\rangle = 0$ and $\langle 1^\star|0\rangle = 0$ is guaranteed by the presence of projectors $Q = Q_0 = 1-P_0$.

Formula (5) re-expresses the original full-space inversion of $\mathcal{M} = 1-K$ in terms of an inversion of the same operator restricted to a subspace. In a way, we just eliminated the $P_0$-projected subspace from our scope completely. Iterating the same construction, we may define the further, biorthogonalized Lanczos basis vectors step-by-step [2],

$$|k+1\rangle = Q_kK|k\rangle, \quad \langle (k+1)^\star| = \langle k^\star|KQ_k, \quad k=1,2,\ldots. \tag{7}$$

Simultaneously, in terms of the new projectors

$$P_k = |k\rangle\frac{1}{\langle k^\star|k\rangle}\langle k^\star|, \qquad Q_k = Q_{k-1}-P_k$$

we may also generalize the abbreviation (6),

$$R_{k+1} = \langle (k+1)^\star|Q_k\frac{1}{Q_k(1-K)Q_k}Q_k|k+1\rangle, \qquad k=0,1,\ldots$$

and immediately re-derive the Horáček and Sasakawa's CF recurrences [4],

$$R_k = \langle k^\star|k\rangle\frac{1}{\langle k^\star|k\rangle - \langle k^\star|K|k\rangle - R_{k+1}}\langle k^\star|k\rangle, \quad k=0,1,\ldots.$$

Here, one introduces the standard CF truncation $R_m = 0$ at a suitable $m \gg 1$ and/or $m\to\infty$ [10] as a practical guide to computations.

## 2.2 The continued fraction representation of Born remainders

In our previous paper [5], a slightly generalized CF prescription was proposed as a particular application of the formalism of ref. [4] to the Born-remainder quantity: In place of the plane waves, just the Born-distorted waves were to be used there. In a slight extension of our previous notation, the formalism is easily described. Abbreviating $\langle u|VK^s \equiv \langle 0^\star(s)|$ and $|0(t)\rangle \equiv K^t\,|u\rangle$, we may mark the subsequent Born approximants by horizontal arrows,

$$\langle u|V|u\rangle \equiv \langle u|T|u\rangle^{(\rightarrow)}, \quad \langle u|V|u\rangle + \langle u|VG_0V|u\rangle \equiv \langle u|T|u\rangle^{(\rightarrow\rightarrow)}, \ \ldots,$$

and write

$$\langle u|T|u\rangle = \langle u|T|u\rangle^{(\overbrace{\rightarrow\rightarrow\ \ldots\ \rightarrow}^{(n-1)-\text{times}})} + R(s,t), \qquad s+t=n, \quad n \geq 0$$

with an explicit Born remainder

$$R(s,t) = R_0(s,t) = \langle 0^\star(s)|\frac{1}{1-K}|0(t)\rangle. \tag{8}$$

For the sake of definiteness, we may fix, say, $s = n-t$ and $t = [n/2]$. In comparison, the only distinction between eqs. (3) and (8) lies in the (inessential) presence of $s$ and $t$. In methodical setting, these integers may be dropped and one may expand the remainders $R(n-t,t)$ in the Horáček and Sasakawa CF spirit again. At an arbitrary pair of integers $s \geq 0$, $t \geq 0$, the Lanczosean recurrences (7) for vectors preserve their form and imply

$$R_k(s,t) = \langle k^\star(s)|k(t)\rangle \frac{1}{\langle k^\star(s)|k(t)\rangle - \langle k^\star(s)|K|k(t)\rangle - R_{k+1}(s,t)} \langle k^\star(s)|k(t)\rangle. \tag{9}$$

For the sake of clarity, let us extend our above Born-approximation convention and mark also each CF Lanczos iteration step by a (superscripted) vertical arrow "$\Downarrow$". With $m$ iterations in eq. (9), we get the final formula

$$\langle u|T|u\rangle \approx \langle u|T|u\rangle^{(\overbrace{\rightarrow\rightarrow\ \ldots\ \rightarrow}^{(s+t)-\text{times}}\overbrace{\Downarrow\Downarrow\ \ldots\ \Downarrow}^{m-\text{times}})}. \tag{10}$$

In spite of a not too persuasive overall numerical performance, the latter scheme exhibited definite numerical merits in the particular interaction models [5]. Unfortunately, we were unable to find any more flexible (and still viable) iteration scheme at that time, presumably due to an inadequate notation. Now, we are going to fill the gap.

# 3 Proposal: Blended iterations

## 3.1 Notation

With a set of integers

$$\vec{n} \equiv (n_0 \geq 0, m_0 > 0, \ldots, n_j > 0, m_j > 0, \ldots, n_L > 0, m_L \geq 0),$$

let us visualise an iteration pattern with $n_0$ Born steps followed by $m_0$ Lanczos steps, $n_1$ further Born iterations etc,

$$\langle u|T|u\rangle \approx \langle u|T|u\rangle^{(\clubsuit)},$$

$$\clubsuit = \overbrace{\rightarrow\rightarrow \ldots \rightarrow}^{n_0-\text{times}} \overbrace{\Downarrow\Downarrow \ldots \Downarrow}^{m_0-\text{times}} \overbrace{\rightarrow\rightarrow \ldots \rightarrow}^{n_1-\text{times}} \ldots \overbrace{\Downarrow\Downarrow \ldots \Downarrow}^{m_L-\text{times}}.$$

It blends the Born and Lanczos iterations in all the possible ways. At a fixed "order of approximation"

$$N_{(\clubsuit)} = \sum_{i=0}^{L} (n_i + 2m_i),$$

the total number of different blendings (cf. their sample in Table 1) will equal the $(N_{(\clubsuit)} + 1)$-st Fibonacci number [11]. A rich flexibility of the scheme is guaranteed.

For a more explicit description, let us split again $n_p = s_p + t_p$ and introduce a set of the bra and ket vectors numbered as follows,

$$\langle 0^\star(s)[p]|, \quad s = 0, 1, \ldots, s_p, \quad |0(t)[p]\rangle, \quad t = 0, 1, \ldots, t_p,$$
$$\langle k^\star(s_p)[p]|, \quad |k(t_p)[p]\rangle, \quad k = 1, 2, \ldots, m_p,$$
$$p = 0, 1, \ldots, L.$$

In terms of the related projectors

$$P_{k,p}(s_p,t_p) = |k(t_p)[p]\rangle \frac{1}{\langle k^\star(s_p)[p]|k(t_p)[p]\rangle}\langle k^\star(s_p)[p]|$$
$$= Q_{k-1,p}(s_p,t_p) - Q_{k,p}(s_p,t_p), \qquad k = 0,1,\ldots m_p - 1$$

with $Q_{-1,0}(s_0,t_0) \equiv I$ and

$$Q_{-1,p+1}(s_{p+1},t_{p+1}) = Q_{m_p-1,p}(s_p,t_p),$$

we may define these vectors iteratively. The initial choice is imminent,

$$\langle k^\star(s)[0]| \equiv \langle k^\star(s)|, \quad |k(t)[0]\rangle \equiv |k(t)\rangle,$$

with $s = 0,1,\ldots,s_0$ and $t = 0,1,\ldots,t_0$ at $k = 0$ and with $s = s_0$ and $t = t_0$ at $k = 1,2,\ldots,m_0$. It is to be followed by the obvious Born-type recurrent prescription

$$\begin{array}{c}\langle 0^\star(s)[p+1]| = \langle m_p^\star(s_p)[p]|(KQ_{m_p-1,p}(s_p,t_p))^s, \quad s = 0,1,\ldots,s_{p+1},\\ |0(t)[p+1]\rangle = (Q_{m_p-1,p}(s_p,t_p)K)^t|m_p(t_p)[p]\rangle, \quad t = 0,1,\ldots,t_{p+1}\end{array} \tag{11}$$

and its Lanczos-type descendant

$$\begin{array}{c}\langle k^\star(s_{p+1})[p+1]| = \langle (k-1)^\star(s_{p+1})[p+1]|KQ_{k-1,p+1}(s_{p+1},t_{p+1}),\\ |k(t_{p+1})[p+1]\rangle = Q_{k-1,p+1}(s_{p+1},t_{p+1})K|(k-1)(t_{p+1})[p+1]\rangle,\\ k = 1,2,\ldots,m_{p+1}\end{array}$$

at all the additional indices $p = 0,1,\ldots,L-1$.

The only really new technicality is a switch between the two types of iterations. In place of the standard CF termination $R_m = 0$ (applicable here at $p = L$ and $m = m_p$ only), we have to return to the explicit definition

$$R_{k,p}(s_p,t_p) =$$
$$= \langle k^\star(s_p)[p]|Q_{k-1,p}(s_p,t_p)\frac{1}{Q_{k-1,p}(s_p,t_p)(1-K)Q_{k-1,p}(s_p,t_p)}Q_{k-1,p}(s_p,t_p)|k(t_p)[p]\rangle$$

of the Lanczos-type remainder. At $k = m_p$ and $p < L$, its nonlinear iterative representation (9) changes into the horizontal Born-type expansion,

$$R_{m_p,p}(s_p,t_p) = \langle 0^\star(0)[p+1]|0(0)[p+1]\rangle + \langle 0^\star(1)[p+1]|0(0)[p+1]\rangle + \ldots.$$

With the definitions (11), only the next Born residual term

$$R_{0,p+1}(s_{p+1},t_{p+1}) =$$

$$= \langle 0^\star(s_{p+1})[p+1]|\frac{1}{1-Q_{m_p-1}(s_p,t_p)KQ_{m_p-1}(s_p,t_p)}|0(t_{p+1})[p+1]\rangle$$

becomes iterated in the vertical direction, in the way discussed in sect. 2.2.

### 3.2 A few remarks on precision

We have seen that the kernels $K$ with small eigenvalues imply the unambiguous preferrence of the Born iterations; the degree of accuracy may be predicted from our knowledge of the maximal eigenvalue. Under the more realistic assumption

$$|\varepsilon_j| > 1,\ j = 0, 1, \ldots, \mathcal{N},\quad \mathcal{N} > 0$$

the purely Born prescription breaks down and the properties of eigenvectors start playing an important role as well. Thus, in the purely CF prescription of ref. [4], the Lanczosean basis vectors (7) rotate closer and closer to the single, highest-weight eigenvector of $K$. Their overlaps with the potential $V$ and original input $|u\rangle$ (often, a plane wave) will carry the most relevant information for an a priori estimate of precision. A rigorous analysis becomes feasible for the separable interaction models where the CF algorithm terminates [6].

The simplest possible superposition (10) of the Born + CF step in ref. [5] exemplifies the first nontrivial beakdown of dichotomy (3) versus (2). After a "downwards" generation of some $n$ Born and $m$ Lanczos basis vectors, the computations proceed in an opposite direction. The vertical "upwards" iterations of the CF denominators are initiated within a $Q_m$-projected subspace, by a trivial remainder $R_m = 0$. The appropriate insertions produce the final approximate $T$-matrix. Unless a pre-determined precision is achieved, the whole procedure is iterated at the higher $n$'s and/or $m$'s. A thorough analysis of convergence has been performed in ref. [5]: In practice, one is expected to work in an adaptive regime – a numerical $n$- and/or $m$-independent result is sought at the still not too large $n$'s and $m$'s.

Within the present, fully universal formalism, the horizontal iterations may be expected to suppress the small-$\varepsilon$ components of the basis. During the vertical steps, the rotation and renormalization of these vectors will take place in general. This enables us to achieve convergence for various forms of the decomposition (4) of the kernel $K$.

A priori, within the light of our preceding analysis, the next-to-simplest, Born-initiated CF formulae

$$\langle u|T|u\rangle \approx \langle u|T|u\rangle^{(\overbrace{\Downarrow\Downarrow\ldots\Downarrow}^{m-\text{times}}\overbrace{\rightarrow\rightarrow\ldots\rightarrow}^{n-\text{times}})} \tag{12}$$

should be considered first of all. They offer a construction which pre-processes the $K$'s as if they were separable operators, i.e., via a CF inversion formula. Then, they Born-eliminate all the remaining (say, infinitely many) small-$\varepsilon$ components of $K$ in the second step, within a subspace. This seems adequate in all the situations where only a few overlaps $\langle 0^\star(0)|f_j\rangle$ dominate, $j < \mathcal{N}$. In such a case, the initial Born iterations become unnecessary or even counter-productive. At the same time, a few initial CF iterations accompanied by a later (or intermediate) inclusion of Born corrections would be definitely an improvement.

The complete separation of the Born/CF iterations seems to be a weak point of all the preceding prescriptions. In between all these extremes, one finds much more blends of the Born (= "horizontal") *plus* Lanczos (= "vertical") iterations of course. A priori, the rotations and multiplicative suppression may be expected to complement each other. Quite naturally, one may also expect that, for some complicated $K$, the horizontal and vertical iterations contribute in effect with some fixed integer weights $i$ and $j$. Under such a hypothesis, our final recommendation would read

$$\clubsuit = \overbrace{\rightarrow\rightarrow\ldots\rightarrow}^{i-\text{times}}\overbrace{\Downarrow\Downarrow\ldots\Downarrow}^{j-\text{times}}\overbrace{\rightarrow\rightarrow\ldots\rightarrow}^{i-\text{times}}\ldots\overbrace{\Downarrow\Downarrow\ldots\Downarrow}^{j-\text{times}}. \tag{13}$$

The idea of such a regular horizontal/vertical iterative interplay is exciting. Its rigorous mathematical foundation seems difficult, but its practical implementation is straightforward (a similar transformation is often used in the theory of ordinary analytic continued fractions [10]).

Of course, the more detailed verification of our expectations already lies far beyond the scope of our present methodical letter. As a sample of the related technicalities (or a hint for applications), we may recall our mathematically more detailed study of convergence of iterations by means of the so called fixed points [12].

# 4 Summary

Two methods of solution of the Lippmann-Schwinger equations (namely, the method of continued fractions [4] and its Born-remainder generalization [5]) were interpreted here as special cases of a single prescription. Two ideas were employed. Firstly, we noticed that both the quoted approaches admit a re-interpretation via a concept of bi-orthogonality. Thus, we introduced certain auxiliary asymmetric projectors $P \neq P^+$ and re-derived both these "vertical-iteration" algorithms as two different versions of the well known Lanczos technique. Secondly, moving beyond the latter framework, we noticed that a Born-like "horizontal" re-arrangement of the Lanczos remainder may be performed at any intermediate vertical iteration step. A maximal flexibility is achieved in this way: The formalism might compete with the standard Padé resummations of the Born series in practice.

The prospective phenomenological applications of the present formalism may be expected to involve the areas where both the pure Born and pure CF iterations failed or gave an unsatisfactory rate of convergence. In all such cases, our present method offers a new hope. Our notation is intended to help in the related numerical work – a transition from the purely CF algorithms to their CF-like descendants (13) is not difficult.

For the sake of clarity, our discussion was aimed at the diagonal $T$-matrix elements. Nevertheless, it is worth noticing that the more realistic nondiagonal and coupled-channel algorithms represent just an extremely straightforward generalization, fully compatible with the present notation conventions as well. All the necessary details may be found in our older comment [13].

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Table 1. The complete list of the first few approximants $\langle u|T|u\rangle^{(\clubsuit)}$.

| the order of approximation $N_{(\clubsuit)}$ | $\clubsuit$ | | | | |
|---|---|---|---|---|---|
| 1 | → | | | | |
| 2 | →→ | ⇓ | | | |
| 3 | →→→ | →⇓ | ⇓→ | | |
| 4 | →→→→ | →→⇓ | →⇓→ | ⇓→→ | ⇓⇓ |
| 5 | →→→→→ | →→→⇓ | →→⇓→ | →⇓→→ | ⇓→→→ |
| | →⇓⇓ | ⇓→⇓ | ⇓⇓→ | | |
| 6 | →→→→→→ | →→→→⇓ | →→→⇓→ | →→⇓→→ | →⇓→→→ |
| | ⇓→→→→ | →→⇓⇓ | →⇓→⇓ | ⇓→→⇓ | →⇓⇓→ |
| | ⇓→⇓→ | ⇓⇓→→ | ⇓⇓⇓ | | |