Iterative solutions of the Lippmann-Schwinger–type equations

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The remainder $R_{(t)}$ of the Born series $\langle u \mid v \rangle + \langle u \mid K \mid v \rangle + \cdots + \langle u \mid K^{t-1} \mid v \rangle + R_{(t)}$ is given an analytic continued-fractional form. The resulting formula is tested on a few schematic examples and recommended as a combined perturbative and algebraic method applicable to various scattering problems.

I. INTRODUCTION

In atomic and molecular physics, the description of scattering is often based on the one- or quasi-one-body Lippmann-Schwinger equation

$$| \phi \rangle = | v \rangle + K | \phi \rangle \ . \tag{1.1}$$

For example, from the Hamiltonian $H = H_0 + U$ (H_0 is the Hamiltonian for free motion), the reaction-matrix definition of phase shifts

$$\tan\delta_l = \langle u \mid \phi \rangle, \quad | u \rangle = U | v \rangle \tag{1.2}$$

may be derived.[1] With the stationary wave $| v \rangle$ and kernel $K = GU$ [$G = P/(E - H_0)$], Eq. (1.1) has a variety of available methods of solution.[1,2]

In a more complex (few-body, multiparticle) context, the scattering equations (e.g., of Faddejev type) still preserve their form (1.1). Its iterative modifications

$$| \phi \rangle = | v \rangle + \cdots + K^{t-1} | v \rangle + K^t | \phi \rangle \tag{1.3}$$

may be used to convert the kernel into a well-defined operator.[1] In this context, it is natural[3] to complement also the standard solution methods by the iterative ones.

Usually, the interative methods[1–8] of solving (1.1) proceed in one of the following two ways:

(a) The $t \to \infty$ limit of (1.3) is accepted as a suitable formal (Born or von Neumann) power-series solution of (1.1),

(b) The $t = 0$ form of (1.3)

$$| \phi \rangle = (1 - K)^{-1} | v \rangle \tag{1.4}$$

is treated by an algebraic inversion. In the present paper, we intend to combine both these techniques.

We shall start from (1.2) and (1.3),

$$\langle u \mid \phi \rangle = \langle u \mid v \rangle + \langle u \mid K \mid v \rangle + \cdots \tag{1.5}$$

and notice that our ability to compute the moments

$$\langle u \mid K^n \mid v \rangle, \quad n \le M \le \infty \tag{1.6}$$

suffices for a numerical determination of the observable quantities. Thus, in a purely mathematical setting, we may consider simply the infinite power series (1.5) replaced by its various algebraic,[4–6] continued-fractional,[7–9] and Padé[10] equivalents. Here, we shall pay attention to the continued-fractional formulas only.

Our main idea is based on the algebraic identity

$$| \phi \rangle = | v \rangle + K | v \rangle + \cdots + K^{t-1} | v \rangle + \frac{K^t}{1-K} | v \rangle \ , \quad t \ge 0 \ . \tag{1.7}$$

Preserving the perturbative tth Born approximation unchanged, we shall invert the remainder term algebraically. The algorithm will be tested on a few schematic models. In comparison with the $t = 0$ techniques,[3–8] we shall see that an optimal choice of $t \neq 0$ may exist, and analyze how it may lead to a significant improvement of approximations generated, e.g., from a finite number $M < \infty$ of moments (1.6).

Our considerations start in Sec. II. A thorough discussion of the $t \to \infty$ convergence and an algorithmic reformulation of the exact $t < \infty$ termination condition (1.7) are presented there. In Sec. III, this is followed by an analysis of the resulting continued-fractional resummations of (1.5) and by a few comments on their extension to the coupled channels. The numerical tests and illustrations are given in Sec. IV. Finally, the properties and merits of the whole method are summarized in Sec. V.

II. REMAINDER IN THE BORN SERIES

A. Convergence

In atomic physics as well as in the further applications of (1.1), a slow $t \to \infty$ convergence or even divergence of (1.5) may be encountered. For the realistic kernels, the algebraic straightforward inversion of the operator $1 - K$ improves the results significantly.[11] Its applicability is of course limited only by the capacity of the available computers.

Alternatively, we may achieve also a better convergence of (1.5) in a less formal, physically motivated way, by the so-called distorted-wave transformation: When we replace K by a "smaller" operator $K_1 = K - K_0$ in such way that the subtracted auxiliary kernel K_0 remains sufficiently simple, we may define $T = (1 - K_0)^{-1/2}$ and reinterpret (1.1)–(1.7) with $| \phi' \rangle = T^{-1} | \phi \rangle$, $| v' \rangle = T | v \rangle$, and

$K'=TK_1T$ as equations valid for the new, primed quantities. The definition $\langle u'|=\langle u|T$ is to be added for the sake of completeness.

From the purely formal point of view, we may often expect that the kernel K is compact, i.e.,[1]

$$K\approx\sum_n |\chi_n\rangle\alpha_n\langle\chi_n|, \quad \alpha_n\to 0, \quad n\to\infty .$$

Then, in a slightly changed notation with

$$K\approx K^{(p,r)}=\sum_{m=2}^{p+1}|m\rangle\varepsilon_m\left\langle m\right| + \sum_{n=2}^{r+1}\left|\tilde{n}\right\rangle\eta_n\langle\tilde{n}| ,$$

$$|\varepsilon_m|<1, \quad |\eta_n|\geq 1, \quad p\leq\infty, \quad r<\infty \qquad (2.1)$$

let us denote the tilded sum by the symbol K_d and notice that the above-mentioned distortion operator K_0 must be a sum of K_d with an arbitrary (or zero) part of $K-K_d=K_c$. Only this may guarantee the convergence of the primed Born series.

An exact knowledge of all the tilded vectors $|\tilde{n}\rangle$ and divergence-causing coefficients η_n is not always available. Then, whenever we compute, in the spirit of (1.2), the matrix elements of the type

$$R=\langle v|K^t/(1-K)|v\rangle ,$$

a necessary and sufficient condition of convergence $R\to 0$ for $t\to\infty$ is merely a disappearance of the overlaps $\langle\tilde{n}|v\rangle$. Vice versa, whenever $\langle\tilde{n}|v\rangle\neq 0$, say, due to the numerical errors, we cannot identify R with its convergent part $R_c=\langle v|K_c^t/(1-K_c)|v\rangle$ and get $R\approx R_d=\langle v|K_d^t/(1-K_d)|v\rangle$ for a large number t of iterations.

In Table I, the interplay between our choice of $t\gg 1$ and the magnitude of errors $\langle\tilde{n}|v\rangle\neq 0$ (i.e., a quality of distorsion) is studied numerically. We employ the three schematic operators $K=K_i^{(p,r)}$ with the orthogonal (biorthogonal) eigenvectors and typical spectra of the type (2.1),

$$\varepsilon_m=1/m, \quad \eta_n=n, \quad i=1 ,$$

$$\varepsilon_m=1/m^2, \quad \eta_n=n^2, \quad i=2 ,$$

$$\varepsilon_m=1/\sqrt{m}, \quad \eta_n=\sqrt{n}, \quad i=3 .$$

Besides a reasonable degeneracy of the $|\varepsilon|<1$ levels,

$$\langle m|v\rangle=m, \quad i=1,3 ,$$

$$\langle m|v\rangle=m^2, \quad i=2 ,$$

we shall simulate here also an approximate distorted-wave elimination of the large components from K, which is less and more precise, respectively,

$$\langle\tilde{n}|v\rangle=1/n, \quad i=1,3 ,$$

$$\langle\tilde{n}|v\rangle=1/n^2, \quad i=2 .$$

For $\langle\tilde{n}|v\rangle\equiv 0$ we would get $R=R_c$ and the remainder would converge to zero with increasing t. An inclusion of errors causes the divergence at large t, $R\sim R_d$. An "optimal" choice of $t=t^*$ (such that $|R_c|\sim|R_d|$) is seen to depend on the quality of distortion ($t^*=3$ for K_1, $t^*=5$ for K_2) as well as on the spectrum of K ($t^*=5$ for K_3). Thus, we may expect that it will be difficult to determine the best number of iterations t^* *a priori*. In the practical computations, a reliable suppression or estimate of the remainder seems to be indispensable.

B. Rearrangements

In Eq. (1.3), let us denote $|v\rangle=|0\rangle$ and define the auxiliary new vectors as arbitrary linear combinations of the old Born components of $|\phi\rangle$,

$$|1\rangle=\frac{1}{B_0}(K|0\rangle-|0\rangle-|0\rangle A_0) ,$$

$$|2\rangle=\frac{1}{B_1}(K|1\rangle-|0\rangle C_1-|1\rangle A_1), \ldots .$$

TABLE I. Convergent and divergent components of Born remainder $R=\langle v|K^t/(1-K)|v\rangle=R_c+R_d$ for $K=K_i^{(9,4)}$, $i=1-3$ and $t=1-5$ (notation $4.3[3]\equiv 4.3\times 10^3$, etc.).

i	t	R_c	R_d	$R_c^2+R_d^2$	R_c/R_d
1	1	65.8	−0.8	4.3[3]	−82.3
	2	11.8	−2.1	144.3	−5.7
	3	2.8	−6.1	45.0	−0.5
	4	0.90	−20.1	404.1	−0.04
	5	0.35	−74.1	5.5[3]	−0.005
2	1	3.4[3]	−0.15	1.2[7]	−2.3[4]
	2	449.8	−0.34	2.0[5]	−1.3[3]
	3	65.8	−0.80	4.3[3]	−82.3
	4	11.8	−2.1	144.2	−5.7
	5	2.8	−6.1	45.0	−0.46
3	1	234.5	−1.3	5.5[4]	−178.5
	2	92.9	−2.1	8.6[3]	−44.8
	3	38.9	−3.4	1.5[3]	−11.6
	4	17.4	−5.6	333.9	−3.1
	5	8.4	−9.6	162.4	−0.87

In the simplest nontrivial case with the three groups A_{k-1}, B_{k-1} and C_{k-1} ($C_0=0$) of the arbitrary parameters, we shall have

$$|k\rangle=(K|k-1\rangle-|k-1\rangle A_{k-1}-|k-2\rangle C_{k-1})/B_{k-1}\,,\quad k=1,2,\ldots\,. \tag{2.2}$$

The assumption[8]

$$|\phi\rangle=\frac{1}{1-K}|0\rangle=|0\rangle F_0+|1\rangle F_1B_0F_0+\cdots \tag{2.3}$$

may be then made formally, with an unspecified initial choice of $F_0\neq 0$ and with the recurrent definition of the remaining coefficients

$$\frac{1}{F_k}=1-A_k-C_{k+1}F_{k+1}B_k,\quad k=0,1,\ldots\,. \tag{2.4}$$

Indeed, Eq. (2.3) represents an algebraic identity since

$$|0\rangle=(1-K)(|0\rangle F_0+|1\rangle F_1B_0F_0+|2\rangle F_2B_1F_1B_0F_0+\cdots)\,,$$

i.e.,

$$\begin{aligned}0=&|0\rangle(-1+F_0-A_0F_0-C_1F_1B_0F_0)\\&+|1\rangle(F_1B_0F_0-B_0F_0-A_1F_1B_0F_0-C_2F_2B_1F_1B_0F_0)\\&+\cdots\end{aligned}$$

which is satisfied as a consequence of (2.4). Thus, Eq. (2.3) may be employed and interpreted as a general rearrangement of the $t=\infty$ Born series (1.3), induced by the reparametrization (2.2).

It is rather puzzling to notice that in (2.3) and (2.4), an initial value of f_0 may be arbitrary. An explanation lies in the infinite dimensionality of the rearrangement (2.2). In practice, a unique specification of F_0 may be related, e.g., to the normalization of $|\phi\rangle$. The corresponding variational specification of the quantities F_k enables one to put $F_N^{(N)}=0$ in the limit $N\to\infty$ and to call $F_0=F_0^{(\infty)}$ simply an analytic continued fraction. In Ref. 12, a non-continued-fractional counterexample may be also found, with a nonvariational interpretation of F_k's.

In place of (2.2), we may start also from the more-term rearrangement of the Born states $K^n|v\rangle$. Then, it is possible to partition the set of parameters and to generalize the formulas (2.2)—(2.4) in a rather straightforward way. We recall Ref. 13 for further details.

A rearrangement of (1.5) of any type is always designed to diminish the remainder. In principle, the formulas like (2.2)—(2.4) enable us to accelerate the convergence or even to convert the divergent Born series into its convergent continued-fractional equivalent.

C. An algebraic termination requirement

In the light of (1.2) one of the most natural specifications of the rearrangement [free parameters in (2.2)] should be based on a termination requirement

$$\langle u|\phi\rangle=\langle u|0\rangle F_0+\cdots+\langle u|t\rangle F_tB_{t-1}F_{t-1}B_{t-2}\cdots F_0 \tag{2.5}$$

imposed on the rearranged infinite Born series. Obviously, this formula will be exact if and only if the incomplete orthogonality conditions

$$\langle u|t+j\rangle=0,\quad j=1,2,\ldots \tag{2.6}$$

will guarantee vanishing of all the remaining overlaps. Without any loss of generality, we may also choose

$$\begin{aligned}&B_0=B_1=\cdots=1\,,\\&C_1=C_2=\cdots=C_t=0,\quad A_0=\cdots=A_{t-1}=0\end{aligned} \tag{2.7}$$

and obtain $F_0=F_1=\cdots=F_{t-1}=1$ and the following.

Theorem. The conditions (2.6) and (2.7) fix uniquely all the free parameters A, B, and C in (2.2).

Proof. A multiplication of (2.2) with $k=t+1$ by $\langle u|$ from the left is compatible with (2.6) if and only if

$$\langle u|t\rangle A_t+\langle u|t-1\rangle C_t-\langle u|K|t\rangle=0\,. \tag{2.8}$$

This specifies $A_t=A_t(C_t)$ [$C_t=0$ in the light of (2.7)] and the vector $|t+1\rangle$. Similarly, the $k=t+2$ item of (2.2) gives

$$\langle u|t\rangle C_{t+1}-\langle u|K|t+1\rangle=0 \tag{2.9}$$

and defines a unique value of C_{t+1}.

The remaining items of (2.2) convert the condition (2.6) into a new requirement

$$\langle u|K|t+1+l\rangle=0,\quad l=1,2,\ldots\,. \tag{2.10}$$

Thus, we may replace $\langle u|k\to\langle u|$, $t+1\to t$, $l\to j$ in (2.10) and return precisely to (2.6) again. A repetition of the above construction defines now $A_{t+1}=A_{t+1}(C_{t+1})$, $|t+2\rangle$, and C_{t+2}. Obviously, the rest of the proof proceeds by the mathematical induction. Q.E.D.

From the above construction, we obtain an iterative algorithm implementable easily on the computer. The corresponding formulas

$$C_{t+m+1}=(\langle u|K^m|t+m\rangle)^{-1}\langle u|K^{m+1}|t+m+1\rangle\,, \tag{2.11}$$

$$\begin{aligned}A_{t+m}=&(\langle u|K^m|t+m\rangle)^{-1}\\&\times(\langle u|K^{m+1}|t+m\rangle\\&-\langle u|K^m|t+m-1\rangle C_{t+m}),\quad m=0,1,\ldots\end{aligned}$$

are of course compatible with the general theory of moments.[9]

The overlaps $\langle u|K^{n+1}|m\rangle$ will be zero for $n\geq 0$ and $m>t+n+1$. In our non-orthogonal "basis" set of vectors $|m\rangle$ and dual vectors $\langle u|K^n$, $m,n=0,1,\ldots$, the operator K will be represented by a partitioned Heisenberg matrix. In general, a formal inverse of such a matrix may be constructed by means of the so-called extended continued fractions.[14] A simplification—reduction of the extended to the ordinary analytic continued fractions—necessitates an additional information about the kernel K or, alternatively, a rearrangement of the dual basis states. This will be discussed in the next section.

III. ANALYTIC CONTINUED FRACTIONAL RESUMMATION OF BORN SERIES

A. $t=0$ and a construction of Lanczos bi-orthogonal basis

In accord with our theorem, we may interpret relations (2.2) and their more-term generalizations[13,15] as a rearrangement of the Born states $K^{n+t}|v\rangle$, $n=0,1,\ldots$. We could start also from an arbitrary bra vector $\langle 0^*|=\langle u|K^q$ and generate an alternative set of its rearranged descendants

$$\langle k^*|=\frac{1}{B^*_{k-1}}[\langle(k-1)^*|K-A^*_{k-1}\langle(k-1)^*| - C^*_{k-1}\langle(k-2)^*|], \quad k=1,2,\ldots. \tag{3.1}$$

In analogy with (2.2), they are defined by means of the free parameters.

Both recurrences (2.2) and (3.1) are independent, but in accord with Lanczos,[5,6] we may relate them by a demand of the mutual bi-orthogonality of the resulting two sequences of vectors,

$$\langle m^*|n\rangle=1, \quad m=n \qquad =0, \quad m\neq n\ . \tag{3.2}$$

Such a prescription fixes also all the parameters. Hence, it may be interpreted as a special case of a termination requirement with $t=0$. Vice versa, the terminations of the type (2.6) must follow from (1.7) and from the Lanczos method in principle.

As a method of inversion of an arbitrary operator, the Lanczos procedure appears and reappears in the various contexts and applications.[7,16–18] In the present physical setting, we may prove also the following.

Lemma. With the particular kernel $K=GU$ such that both G and U are Hermitian, the $t=0$ Lanczos construction of a basis reproduces the interative quasiparticle algorithm of Ref. 3.

Proof. Let us summarize first the essence of the continued fractional technique of Ref. 3. Defining $K_{M+1}=GU_{M+1}$ where $U=U_0$, $|v\rangle=|v_0\rangle$, and

$$U_{M+1}=U_M-U_M|v_M\rangle(\langle v_M|U_M|v_M\rangle)^{-1}\langle v_M|U_m\ , \qquad |v_{M+1}\rangle=GU_M|v_M\rangle, \quad M=0,1,\ldots \tag{3.3}$$

we may denote $|w_0\rangle=0$, $|w_{M+1}\rangle=U_M|v_M\rangle$, $M=0,1,\ldots$ and compute the matrix $B_0=\langle w_1|\phi\rangle$ (1.2) from the easily derived recurrences

$$B_M=\langle w_M|v_M\rangle+\langle w_{M+1}|v_M\rangle D_M\langle w_{M+1}|v_M\rangle\ , \qquad D_M=(\langle w_{M+1}|v_M\rangle-B_{M+1})^{-1}, \quad M=0,1,\ldots. \tag{3.4}$$

Now, it is sufficient to notice that, due to the Hermiticity, the overlaps of the vectors $|v_m\rangle$ and $|w_n\rangle$ are symmetric,

$$\langle w_m|v_n\rangle=\langle w_m|G|w_n\rangle=\langle w_n|v_m\rangle\ . \tag{3.5}$$

For $|m-n|>1$, they are equal to zero.[3] Since

$$U=|w_1\rangle\frac{1}{\langle w_1|v_0\rangle}\langle w_1|+|w_2\rangle\frac{1}{\langle w_2|v_1\rangle}\langle w_2)+\cdots \tag{3.6}$$

we get

$$UG|w_1\rangle=|w_1\rangle A_0+|w_2\rangle\ , \tag{3.7}$$

$$UG|w_{m+2}\rangle=|w_{m+1}\rangle C_{m+1}+|w_{m+2}\rangle A_{m+1}+|w_{m+3}\rangle, \quad m=0,1,\ldots,$$

where

$$A_0=\frac{1}{\langle w_1|v_0\rangle}\langle w_1|G|w_1\rangle\ , \qquad A_{m+1}=\frac{1}{\langle w_{m+2}|G|w_{m+1}\rangle}\langle w_{m+2}|G|w_{m+2}\rangle \tag{3.8}$$

and

$$C_1=\frac{1}{\langle w_1|v_0\rangle}\langle w_1|G|w_2\rangle\ , \qquad C_{m+2}=\frac{1}{\langle w_{m+2}|G|w_{m+1}\rangle}\langle w_{m+2}|G|w_{m+3}\rangle\ . \tag{3.9}$$

Thus, the vectors $|w_1\rangle$, $|w_2\rangle,\ldots$ satisfy the three-term recurrences of the type (2.2).

Next, we may construct a set of the bra vectors

$$\langle 1^*|=\langle v|, \quad \langle 2^*|=\langle 1^*|UG-A^*_0\langle 1^*|,\ldots$$

bi-orthogonal to $|w\rangle$'s. In accord with (3.2), we get

$$A^*_0=\langle 1^*|UG|w_1\rangle/\langle 1^*|w_1\rangle=A_0\ ,$$

i.e., $\langle 2^*|U=\langle w_2|$, etc. We may conclude that the set $|w_1\rangle$, $|w_2\rangle$, $|w_3\rangle,\ldots$ coincides precisely with the $t=0$ Lanczos ket basis. The proof of equivalence of the two methods is completed. It remains for us only to notice that a use of (3.7) and of the Lanczos bra states $\langle 1^*|,\langle 2^*|,\langle 3^*|,\ldots$ would make the explicit construction of the full "weakened" kernels K_{M+1} or U_{M+1} (motivated[3,4] by the physical quasiparticle interpretation of the algorithm) redundant. Q.E.D.

B. Continued fractional expansion of the tth Born remainder

The physical quantity $R_{(0)}=\langle v|U/(1-GU)|v\rangle$ in the alternating arrangements

$$R_{(0)}=\langle v'|(1-G')^{-1}|v'\rangle=\langle v''|U'(1-U')^{-1}|v''\rangle\ , \qquad |v'\rangle=|\sqrt{U}|v\rangle, \quad |v''\rangle=G^{-1/2}|v\rangle\ , \qquad G'=\sqrt{U}G\sqrt{U}, \quad U'=\sqrt{G}U\sqrt{G} \tag{3.10}$$

may be treated algebraically as a Lanczos inversion with $q=0$ or 1, respectively. In both cases, the operator square roots need not be unique[1] and we invert $1-GU$ without any preliminary iterations (1.7).

From the purely formal point of view, our termination algorithm of Sec. II C will be fully equivalent to the Lanc-

zos continued-fractional inversion prescription (or Padé techniques[19,20]), applied directly to the remainders

$$R_{(t)}=\langle v \mid U(GU)^t/(1-GU) \mid v\rangle, \quad t\geq 0 . \tag{3.11}$$

A priori, a preference of $t\neq 0$ may prove to be useful at least because of the following two reasons.

(1) It is well known that the Lanczos algorithm suffers from a loss of precision causing a need to compute a square root of a negative number.[6] Such a possibility appears during the renormalizations ($B_m=\text{const}$) $\rightarrow$($\langle m \mid m\rangle=\text{const}$). In the present termination constructions, it occurs also for $t=0$ but it is absent for $t\geq 1$ (cf. once more the proof of theorem in Sec. II C).

(2) Trivially, assuming that an amount of information about the kernel K is restricted to a finite number $M=2N+t-1$ of the available moments (1.6), we must use at least $t=1$ for any even M.

An *a posteriori* support of a nonzero parameter t will stem from the numerical tests in Sec. IV below.

C. Transition to the coupled channels

A coupled-channel extension of the present formalism is straightforward and a use of the partitioning[4,13,15] enables us to preserve even the notation (formulas). In brief, we may extend easily the validity of all the above considerations with the channel-indexed vectors

$$|v\rangle=\{|v\rangle^{(1)}, |v\rangle^{(2)}, \ldots, |v\rangle^{(s)}\} ,$$

recurrences of a partitioned three-term form

$$K|m-1\rangle^{(i)}=\sum_{j=1}^{s}[|m-2\rangle^{(j)}C_{m-1}^{(j,i)} + |m-1\rangle^{(j)}A_{m-1}^{(j,i)}+|m\rangle^{(j)}B_{m-1}^{(j,i)}] ,$$

$$i=1,2,\ldots,s, \quad \det B_{m-1}\neq 0 , \tag{3.12}$$

etc. Then, we may employ the standard summation conventions and omit the explicit channel indices again. Up to a necessity to preserve the ordering of the noncommutative matrices, all the formulas will preserve the same form as above.

On a less formal level, Eq. (3.12) represents in general the $3s$-term recurrences now. As a definition of the new states $|m\rangle^{(i)}$, it is slightly ambiguous and necessitates an $(s\times s)$-dimensional inversion of B_{m-1}. Hence, unless we decide to choose $B_{m-1}=1$ again, we may generate recurrently the $s\times s$ matrices $\langle n \mid m\rangle B_{m-1}$ and factorize them into the products of the respective "canonical" lower and upper triangular matrices $\langle n \mid m\rangle$ and B_{m-1}. In this way, when working with the manifestly Hermitian matrices [e.g., in the notation of Eq. (3.10)], our termination condition (2.6) [+ a choice (2.7) of B's] may be replaced by a more specific and two-sided "partial-orthogonality" requirement

$$\begin{aligned} {}^{(i)}\langle n \mid m\rangle^{(j)}&=0, \quad |m-n|>t \\ &=0, \quad m-n=t, \quad i<j \\ &=0, \quad -m+n=t, \quad i>j . \end{aligned} \tag{3.13}$$

Such a renormalization ($B_{m-1}\neq 1$) shortens (3.12) to mere $(2s+1)$-term recurrences and modifies only slightly the corresponding recurrent algorithm.

Another specific feature of the $s>1$ case is a difficulty to keep the norm of the higher states $|m\rangle^{(i)}$ under control. Hence, it is useful to complement (3.13) by

$${}^{(i)}\langle n \mid m\rangle^{(j)}=1, \quad |m-n|=t, \quad i=j . \tag{3.14}$$

This "partial normalization" converts the family of overlaps into a $(2st+1)$-diagonal band matrix with a pair of the unit outer diagonals.

Of course, the coupled-channel continued fractions remain still $(s\times s)$ dimensional. With $s>1$, their formal properties are less understood from the purely mathematical point of view. These details[4,13] are omitted here.

TABLE II. Born remainder as a continued fraction ($K=K_i^{[4,2)}$, $t=3$).

Indices			Coefficients		Approximants
i	n	N	A_n	B_nC_{n+1}	$F_0^{(N)}$
4	0	4	4.209	2.222	−0.18
	1	5	2.083	0.379	−0.096
	2	6	1.446	0.124	−0.0691
	3	7	1.089	0.045	−0.070 159
	4	∞	0.882	0.015	−0.070 139
5	0	4	4.729	0.827	−0.289
	1	5	1.869	0.267	−0.2740
	2	6	1.283	0.096	−0.271 51
	3	7	1.013	0.036	−0.271 719
	4	∞	0.841	0.012	−0.271 722
6	0	1	4.817	0.517	−0.2967
	1	2	2.154	0.047	−0.294 287
	2	3	0.400	0.003	−0.294 271 362
	3	4	0.123	0.000	−0.294 271 347
	4	∞	0.034	0.002	−0.294 271 347

TABLE III. Estimated number $\chi_{N,t}=-\log_{10}|F_0^{(N)}/F_0^{(\infty)}-1|$ of significant digits in the Nth continued fractional approximation of the Born remainder $R=\langle v|K^t/(1-K)|v\rangle$, $K=K_6^{(4,2)}$.

N		1	2	3	4	5
t	R			$\chi_{N,t}$		
0	14.374	0.1	0.7	2.7	5.9	≥ 9
1	−9.624	−0.5	1.3	3.7	7.0	≥ 8
2	−39.958	1.0	2.8	5.5	≥ 9	
3	−156.621	2.1	4.3	7.3	≥ 9	
4	−681.857	3.1	5.9	≥ 9		
5	−3252.945	4.2	7.3	≥ 9		

IV. NUMERICAL TESTS

Let us use the termination algorithm of Sec. II C and denote $R_{(t)}=\lim_{N\to\infty}R_{(t)}^{(N)}$, $R_{(t)}^{(N)}=\langle v|U(GU)^t|v\rangle F_0^{(N)}$ where

$$F_k^{(N)}=(1-A_k-B_kF_{k+1}^{(N)}C_{k+1})^{-1},\quad k=0,1,\ldots,N-1$$
$$F_N^{(N)}=\cdots=0 \tag{4.1}$$

are the finite continued-fractional approximants.[16] Their good $N\to\infty$ convergence is well known.[3] Moreover, for the finite-dimensional kernels (2.1) (with $p<\infty$) they will even provide an exact answer at a finite $N=N_0=p+r+1$. With $N_0=7$, this is illustrated in Table II. The "$N=\infty$" item is also added to illustrate a complete absence of the $N>N_0$ instabilities, which is compatible with our remark (1) made in Sec. III B above.

In the testing models K_4–K_6, we have preserved the simplicity of K_1–K_3 and used the modified spectra

$$\eta_1=5,\ \eta_2=2,\ r\leq 2,\ \varepsilon_m=\frac{10}{3m^3+2},\ m\geq 2,\ i=6$$
$$\eta_3=1.25,\ r\leq 3,\ \varepsilon_m=\frac{10}{3m+5},\ m\geq 2,\ i=4,5 \tag{4.2}$$

with fewer symmetries and very small eigenvalues in the latter $i=6$ case. Also, we have omitted now the distortions and simplified the overlaps

$$\langle\tilde{n}|v\rangle=n,\quad n=2,3,4$$
$$\langle m|v\rangle=m+3,\quad m\geq 2,\quad i=4 \tag{4.3}$$
$$\langle\tilde{n}|v\rangle=\langle m|v\rangle=2,\quad i=5,6\ .$$

concentrating our attention on the relevance of the spectra.

When we vary the parameter t, the overall convergence pattern may be read out of Table III. The precision of $F_0^{(N)}$ increases with the increasing t, due to the relative

TABLE IV. Variation of an optimal $t=t^*$. Relative errors $|(R^{(N)}-R^{(\infty)})/R^{(\infty)}|$ are tabulated for the variable $M=2N+t-1$ and $K=K_2^{(6-r,r)}$. † marks a need for the double precision arithmetic.

r	M \ t	0	1	2	3	4	5	6
2	0		0.56[1]					
	1	1.8[−3]*		4.0[−3]				
	2		1.9[−4]		0.74[−4]*			
	3	0.50[−1]		1.2[−4]*		1.1[−2]		
	4		4.7[−4]*		1.2[−3]		0.79[−1]	
	5	2.4[−5]		3.3[−6]*		1.9[−4]		0.66[0]
	6		2.8[−6]*		4.8[−5]		4.1[−5]	
	7	3.1[−8]		1.1[−8]*		1.3[−6]		0.92[−5]
	8		2.0[−9]*		2.3[−8]		1.3[−7]	
	9	0.94[−9]		0.72[−11]*		1.7[−9]		1.9[−8]
0	0		3.0[−2]					
	1	0.53[−5]*		1.4[−3]				
	2		0.59[−6]*		1.3[−4]			
	3	1.3[−8]*		0.53[−7]		2.2[−5]		
	4		0.95[−9]*		4.0[−9]		4.7[−6]	
	5	4.8[−10]		0.58[−10]*		2.6[−10]		1.1[−6]
	6		1.4[−11]		3.0[−12]		1.5[−1]*	
	7	4.8[−10]†		0.62[−12]		1.7[−13]		3.0[−14]*
	8		1.4[−11]†		053[−13]		1.1[−15]*	

TABLE V. Patterns of convergence of the various resummed divergent Born series. ‡ denotes the nondecreasing errors.

M \ t	0	1	2	3	4	5
			(a) $K=K_2^{(9,2)}$			
0		1.5[−2]				
1	1.9[−4]		3.5[−4]			
2		1.8[−5]		1.1[−4]		
3	1.0[−2]‡		3.2[−4]		1.0[−3]	
4		1.6[−5]		3.1[−5]		1.2[−2]
5	0.60[−4]		4.5[−5]		3.7[−5]	
6		4.3[−5]‡		0.73[−4]‡		1.9[−4]
7	3.4[−6]		0.56[−5]		0.82[−5]	
8		3.9[−7]		0.74[−6]		1.9[−6]
9	1.4[−8]		3.4[−8]		0.67[−7]	
10		1.3[−9]		2.1[−9]		0.80[−8]
11	4.9[−10]		0.93[−11]		2.7[−10]	
12		1.5[−11]		1.9[−10]		3.2[−9]
			(b) $K=K_2^{(9,4)}$			
0		1.5[−2]				
1	1.7[−4]		3.5[−4]			
2		3.9[−5]		4.5[−3]		
3	3.7[−4]‡		4.9[−2]‡		2.0[−3]	
4		2.2[−6]		1.4[−5]		
5	2.6[−4]‡		4.0[−3]‡		0.99[−4]	
6		2.4[−5]‡		4.2[−5]		
7	3.6[−5]		0.82[−3]‡		2.2[−5]	
8		0.53[−4]‡		0.93[−4]‡		
9	3.7[−6]		1.9[−4]		0.91[−5]	
10		4.2[−7]		0.64[−6]		
11	1.5[−8]		1.1[−6]		0.72[−7]	
12		1.4[−9]		2.3[−9]		
13	0.98[−9]		2.9[−8]		4.1[−8]	
14		1.5[−11]		4.2[−10]		
			(c) $K=K_3^{(9,4)}$			
0		3.8[−1]				
1	1.2[−1]		1.5[−1]			
2		3.0[−2]		0.57[−1]		
3	1.4[−3]		1.0[−2]		1.9[−2]	
4		0.57[−2]		2.9[−3]		
5	0.87[−2]		1.6[−2]‡		2.1[−3]	
6		3.3[−3]		1.1[−1]‡		
7	3.1[−3]‡		0.76[−3]		1.1[−2]‡	
8		0.91[−2]‡		1.3[−3]		
9	0.99[−3]		1.6[−2]‡		4.1[−3]‡	
10		2.6[−4]		3.7[−3]‡		
11	2.3[−3]‡		3.3[−4]		1.5[−3]	
12		2.5[−3]‡		1.1[−3]		
13	1.2[−4]		1.1[−3]‡		3.5[−3]‡	
14		0.61[−4]		4.8[−4]		
15	2.4[−6]		3.1[−5]		2.4[−4]	
16		1.3[−6]		0.84[−5]		
17	0.87[−7]		1.1[−7]		1.1[−5]	
18		0.57[−7]		2.7[−7]		
19	2.5[−7]‡		1.9[−7]‡		1.6[−6]	
20		1.8[−9]		4.9[−8]		
21	1.1[−8]		1.6[−9]		2.3[−8]	
22		1.1[−10]		0.65[−8]		
23	†		1.3[−12]		0.80[−8]	
24		†		1.9[−10]		

suppression of the small eigenvalues in K. In the example $K_6^{(4,2)}$, this is paralleled by a loss of precision caused by the $t\to\infty$ divergence of $R_{(t)}$. Hence, a choice of the optimal t^* is far from being obvious or unique for a fixed input $M=2N+t-1$.

A possible variation in such a choice of t^* is illustrated here in Table IV. In the first part of the table, the remainder $R_{(t)}$ itself diverges, and we find an optimal value of $t=t^*\approx 2$ for $K=K_2^{(4,2)}$. In the second part of Table IV, $R_{(t)}$ (i.e., Born series) converges in the limit $t\to\infty$, and an optimal $t=t^*$ seems to grow with M. A loss of precision (marked by a dagger) appears at some critical truncation $N\approx N^\dagger$ of the continued fractions rather than at the "natural" truncation $M\approx M_0$ of the input information. Hence, the fixed precision of our computers represents a reason for the iterative evaluations of $R_{(0)}$ with the large values of $t=t^*\approx M-\text{const}$.

Once we choose a fixed order t of iterations (1.7) or (2.5), an improvement of precision becomes a purely algebraic matter. The corresponding continued-fractional algorithm is easily implemented on the computer and Tables II–IV may be read also as a representative sample of its $N\to\infty$ convergence.

A priori, one of the main characteristics of the $N\to\infty$ convergence is a number r of the large eigenvalues in $K_i^{(p,r)}$ (2.1). Indeed, for $r=0$ we return to the convergent Born series and have $N\approx\text{const}$ (cf. Table IV). In the methodically more interesting case $r>0$, the vectors $K^n|v\rangle$ become roughly r dimensional for the sufficiently large n. Then, the smooth algebraic continued-fractional convergence at $N\gtrsim r$ is a well-known feature of all the $t=0$ algorithms.[7] A similar phenomenon finds its confirmation also for $t>0$ in Table V here.

Empirically, the restriction $N>N_0(t,r)$ may be replaced by the rule $M>M_0(r)$. In the first two parts of Table V, an oscillation of errors (marked by ‡) disappears for $M>M_0\approx 6$ $(K=K_2^{(9,2)})$ and for $M>M_0\approx 8$ $(K=K_2^{(9,4)})$. The third, "tough" example $K=K_3^{(9,4)}$ with a relatively slow convergence, necessitates $M_0\approx 13$ and exhibits also a reappearance of the small oscillations at $M>M_0$, or a more complex dependence of M_0 on the parity of t. Nevertheless, even this example leads to the quick overall increase of precision for $M>13$.

All the present tests have an emphasized methodical character. Obviously, new features may emerge in a study of the physical systems. This is beyond the scope of the present paper—some particular realistic tests of this type are already under preparation.[15]

V. SUMMARY

We have described a new iterative method of solving the scattering equations. It combines the tth Born approximation with the Nth continued-fractional approximant of its remainder. Since, separately, the corresponding exact $t\to\infty$ (von Neumann) and $N\to\infty$ (Lanczos) limiting transitions are often used in practice, we were interested in their improvement and analysis in the whole two-dimensional t-N plane.

Let us summarize our present conclusions.

(1) The decisive difference has been found between the divergent and convergent behavior in $t\to\infty$. The former case seems to admit a variation of the optimal $t=t^*$ in an interval since the $t\to\infty$ divergence and $N\to\infty$ convergence compensate each other. The $N\to\infty$ convergence proves to be very good for $N\gtrsim N_0$, in accord with the other continued fractional techniques.[7]

(2) The latter ($t\to\infty$)-convergent group of examples supports a preference of an optimal $N=N^*$ and growing $t=t^*$ in practice. The tests indicate a premature computer loss of precision for the smaller t's.

(3) In both cases, a continued-fractional estimate of Born remainder makes the results reliable. An independent variation of t and N may enable one to extract the physical information from the computer input (i.e., from the computed moments of K) in an optimal way.

(4) In a broader methodical context, an analysis of interference between the simple iterations and sophisticated algebraic manipulations proved useful. Their "complementarity" may be expected to manifest itself also in the coupled-channel case described here by means of the matrix continued fractions.

(5) In both the realistic one-channel and coupled-channel calculations, the continued-fractional approach finds its natural extension in a use of the general (possibly, matrix) Padé approximants[10] $[N/N+s]$, s an integer. Indeed, the present continued-fractional remainder $R_{(t)}^{(N)}$ is in fact[17,18] a special Padé approximant with $s=0$. This is a nontrivial relationship since the Padé approximant may also be interpreted as a Schwinger variational expression.[19] Thus, our Born series with analytic continued-fractional remainder $R_{(t)}^{(N)}$ is in fact identical to the variational functional $M_{2t+1,2t+1}^t$ discussed in Ref. 20 (with no initial basis set). This opens a way towards the further analysis: the role of $s\neq 0$ represents an exciting challenge for the further methodical development.

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