Separable expansions of the NN t matrix via exact half-off-the-energy-shell methods

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Recently a method was proposed by which one can obtain rank-1 (for uncoupled channels) and rank-2 (for coupled channels) energy-dependent separable t-matrix representations which are exact on and half off of the energy shell. Fully off shell, this representation, though accurate at low energies, is flawed. For uncoupled channels, if the phase shift passes through zero, the representation has a pathology. Here we investigate two methods which overcome this; one due to Haberzettl which we extend to coupled channels, and the second which is based upon selective combination of the elements of Sturmian expansions. We investigate and compare all methods of separation over a range of energies up to 250 MeV for the $^1S_0$ and $^3S_1$ channels with the Paris interaction. Special attention is paid to the convergence of the higher-order Haberzettl expansion and to the comparison of the extended methods for energies around the zero-phase-shift pathology for the $^1S_0$ channel.

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I. INTRODUCTION

Despite the fact that the three-body problem can be solved exactly [1, 2], separable forms remain essential for solution of many-body problems [3–7]. Even so, it has been known for many years that separable representations of the two-nucleon (NN) t matrix facilitate convenient and quite accurate solutions of the Faddeev equations for bound and scattering three-nucleon problems [8–10]. That spurred studies to find separable representations of most sophisticated, particle exchange model, NN interactions (among which those of the Paris [11] and Bonn [12] groups are noteworthy). One reason for such developments was that phenomenological interactions of the past, while parametrized to give correct on-shell NN t matrices (and so agree with measured NN data) were arbitrary with regard to off-energy-shell properties of the t matrix; properties which are directly involved in three-body problem calculations. It has long been hoped that such dependences, along with determination of realistic three-body forces, would permit the use of data from three-nucleon systems to discriminate between the diverse postulates of the basic NN interaction. Indeed such was the case when the Ernst-Shakin-Thaler (EST) separable expansion procedure [13] was used [14] to define the PEST (for the Paris force) and BEST (for the Bonn force) separable interactions [15, 16] at a low rank (usually ≤ 6). But there are many techniques one can now apply to obtain useful separable representations (of t matrices, for example) and an excellent review of them is to be found in Ref. [17].

Herein we are concerned with two specific methods of defining very low rank (≤ 4) separable expansions of a realistic t matrix, and with the link between those methods. The first, a W-matrix expansion, is based upon the formalism of Bartnik, Haberzettl, and Sandhas [18]. In that formalism, the Lippmann-Schwinger equation is so modified that solutions can be found for both bound and continuum cases in terms of solutions (the W matrices) of nonsingular, real but inhomogeneous integral equations. The relevant t matrix (in each angular momentum channel) is then a rank-1 (uncoupled) or rank-2 (coupled) separable product of (half-off-shell) W matrices plus a remainder matrix [18–20]. All remainder matrices are real and exactly zero half off of the energy shell. For low energies (< 100 MeV in the center of mass), the separable representations of the t matrices obtained by ignoring the remainders is reasonable [20]. Better representations, however, can be obtained by using higher-order W-matrix expansions [21] in which the remainder matrices are iteratively expanded. We demonstrate herein that such is the case. It was also suggested [21] that higher-order expansions would alleviate the singularity effect that occurs when the uncoupled on-shell t matrix is zero. That suggestion is considered herein, along with rank-N W-matrix expansions which can be made for coupled two-nucleon channels as well. For each of those channels, a pathology occurs when the determinant of the coupled matrix on-shell is zero.

The second method of interest, the Sturmian splitting method (referred to hereafter as the SSM), is based upon use of an expansion scheme involving Sturmians [22, 23].

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In this scheme, Sturmian expansions of sufficiently high order (as to reproduce the full t matrices as accurately as one requires) are taken. Then, by simply grouping contributions to each separable representation into a set having attractive character and a set having repulsive character, it is possible to avoid any pathology so defined above. The result is a rank-2 W-like separable interaction for uncoupled channels (rank 4 for coupled channels). As in the original method [18, 20, 21], this remains exact on and half off of the energy shell while also representing the imaginary component of the full t matrices precisely. As we shall show, this scheme can provide good descriptions of the fully-off-shell properties as well.

In the next section we give a brief summary of the W-matrix method [18,20] (WM), and then present its extension to higher rank in a coupled channel formalism with the scheme as presented by Haberzettl [21] (HM) for the uncoupled case. Then, in Sec. III, after a brief description of Sturmian expansions of NN t and K matrices, we present the SSM by which low-rank separable W-like representations of those t matrices can be obtained. Our results are presented and discussed in Sec. IV with emphasis placed upon comparing the results of (low rank) HM calculations with those of the SSM at energies near to zero phase (determinant) pathologies.

II. COUPLED CHANNELS, RANK-N, W-MATRIX THEORY

W-matrix theory is an interesting approach to specifying a separable expansion of NN t matrices (in each two-body channel) in that it gives an energy-dependent representation that is exact both on and half off of the energy shell. The basic theory is that of Bartnik, Haberzettl, and Sandhas [18]. It is similar to a proposition [24] given several years ago, but differs from that scheme by being continuous across positive and negative energies. It has also been extended to describe coupled NN channels [20], in which cases the separable forms have rank 2. They remain exact on and half off shell.

Our interest is to find how good an approximation these separable representations are fully off of the energy shell. Then, there is a nonzero remainder which in all channels is explicitly real and which can be determined, also explicitly, from W-matrix equation solutions. For negative energies, an example of the value of the approximation is its use in evaluation of the triton binding energy. In this circumstance, the "on-shell momentum," k can be treated as a variational parameter. By so doing, a number of studies [25,26] with uncoupled potentials, and one now with coupled interactions [27], have found excellent agreement between exact three-body binding energy calculations and those made using optimal WM separable representations. The optimal choice being with that value of k for which the remainders to the original rank-1 (rank-2) W matrices are minimal.

At low positive energies, the approximation to the fully-off-shell t matrices is quite good [20]. Therefore the method gives separable interactions appropriate for n-d scattering [25] and breakup [28] calculations. However the approximation deteriorates with increasing energy [20] and the method is pathological whenever the associated (on-shell) scattering phase shift in an uncoupled channel vanishes. For coupled channels, a pathology occurs whenever the determinant of the on-shell W matrix is zero; a condition for which the physical observables satisfy [29]

$$\tan^2(2\bar{\epsilon}) = \frac{\tan^2(\bar{\delta}_{J+1}+\bar{\delta}_{J-1}) - \tan^2(\bar{\delta}_{J+1}-\bar{\delta}_{J-1})}{1+\tan^2(\bar{\delta}_{J+1}-\bar{\delta}_{J-1})}\,, \tag{2.1}$$

where the label J refers to the total angular momentum, $\bar{\epsilon}$ is the mixing coefficient, and the Stapp representation is assumed.

But recently, Haberzettl [21] has shown how the remainder matrices in the lowest rank WM approach can in turn be expressed by successive separable expansions. Thereby one can define a rank-N W-matrix theory. He also proposed that expansion to higher rank will "cure" the pathologies. How high a rank one must use in that prescription is then critical for the utility of the W-matrix method. Herein we extend the HM to coupled channels. We begin with a brief review of the basic rank-1 (rank-2 for coupled channels) WM theory [18, 20], not only to define the relevant quantities but also because we have found it convenient to vary the definition of the basic W matrix.

Two-nucleon t matrices are solutions of coupled channel Lippmann-Schwinger equations, viz., for each angular momentum quantum number set (JST)

$$\begin{aligned} t_{LL'}(p',p;E) = {} & V_{LL'}(p',p) \\ & + \sum_l \int_0^\infty \frac{q^2 dq}{(E-q^2)} \\ & \times V_{Ll}(p',q) t_{lL'}(q,p;E). \end{aligned} \tag{2.2}$$

For positive energies, the way the singularity in Eq. (2.2) is handled determines the boundary conditions of the solution of the Lippmann-Schwinger equation in coordinate space. If one performs a complex-plane contour deformation, then Eq. (2.2) yields the standard outgoing transition matrix (the t matrix) if the singularity is passed from below (or equivalently if the pole is slightly moved in the upper half-plane by the substitution $E \to E + i\epsilon$). If the principal value of the singular integral is considered, then the same equation yields the stationary reactance matrix (the K matrix).

It is also possible to offset that singularity by defining a suitably modified inhomogeneous integral equation which is nonsingular. This equation defines the real, nonsingular W-matrix solution whose form for each NN channel (JST) is

$$\begin{aligned} & W_{LL'}(p',p;E) \\ & = V_{LL'}(p',p) \\ & \quad + \sum_l \int_0^\infty \frac{q^2 dq}{(E-q^2)} \{V_{Ll}(p',q) - V_{Ll}(p',k)\} \\ & \quad \times W_{lL'}(q,p;E) \end{aligned} \tag{2.3}$$

differing from the previous specification [18, 20] wherein momentum scaled forms of the interaction were used. Here, $k(=\sqrt{E})$ is the on-shell momentum for positive energies (assuming $\frac{2m}{\hbar^2}=1$) and, as noted previously, for negative energies k can be taken as a variational parameter against which W-matrix equations can be solved to minimize the remainder terms to a separable expansion of the t matrices.

For uncoupled channels ($L=L'$) these are scalar equations while for coupled channels all entities are components of 2×2 matrices. Whichever, straightforward numerical solutions are feasible for the W-matrix equations because the potential terms regularize the pole in the propagator.

Half off the energy shell, the solutions of Eqs. (2.2) and (2.3) are related by

$$t_{LL'}(p',k;E)=\sum_l W_{Ll}(p',k;E)\left\{\mathbf{F}^{-1}(E)\right\}_{lL'}, \tag{2.4}$$

where

$$F_{LL'}(E)=\delta_{LL'}-\int_0^\infty \frac{q^2dq}{(E-q^2)}W_{LL'}(q,k;E) \tag{2.5}$$

and wherein the brackets { } and the bold face notation serve to remind one that, for coupled channels, the inverses are of 2 × 2 matrices.

Since in Eq. (2.4) $t_{LL'}(p',k;E)$ represents the standard t matrix, the singular integral in Eq. (2.5) has to be handled by the corresponding contour deformation method. In such a case, the matrix $F_{ll'}(E)$ is the Jost matrix of the associated two-body problem. If in Eq. (2.4) we consider the reactance matrix $K_{LL'}(p',k;E)$, then the principal value of the singular integral has to be considered in Eq. (2.5), and the matrix $F_{ll'}(E)$ will represent only the *real* part of the associated Jost matrix, namely

$$K_{LL'}(p,k;E)=\sum_l W_{Ll}(p,k;E)\mathrm{Re}[\left\{\mathbf{F}^{-1}(E)\right\}_{lL'}]. \tag{2.6}$$

Fully off the energy shell, the t matrices may be represented in terms of these W-matrix solutions by

$$t_{LL'}(p',p;E)=t^S_{LL'}(p',p;E)+X^{(0)}_{LL'}(p',p;E), \tag{2.7}$$

where the first term has the separable form

$$t^S_{LL'}(p',p;E)=\sum_{ll'} W_{Ll}(p',k;E)\Delta_{ll'}(E)W_{L'l'}(p,k;E), \tag{2.8}$$

with

$$\Delta_{ll'}(E)=\sum_{l''}\left\{\mathbf{W}^{-1}(k,k;E)\right\}_{ll''}\left\{\mathbf{F}^{-1}(E)\right\}_{l'l''}, \tag{2.9}$$

while the second term is the nonseparable remainder defined by

$$\begin{aligned}X^{(0)}_{LL'}(p',p;E) = {} & W_{LL'}(p',p;E)\\ & -\sum_{ll'} W_{Ll}(p',k;E)\\ & \times\left\{\mathbf{W}^{-1}(k,k;E)\right\}_{ll'} W_{l'L'}(k,p;E).\end{aligned} \tag{2.10}$$

This real remainder matrix vanishes identically if either p or p' equals the on-shell momentum value (k) where at half-off shell we have an exact separable representation of the t matrices, t^S, given by Eqs. (2.8) and (2.9). Note that Eq. (2.8) yields equivalently the separable representation of either the standard t matrix or the K matrix, according to whether we interpret $F_{ll''}(E)$ in Eq. (2.9) as the complete Jost matrix or just its real part.

It is also worth noting that, although Eq. (2.8) appears to be rank 4, it can be simplified into rank 2 via diagonalization of Δ, redefining it in Eq. (2.9) as

$$\Delta_{LL'}(E)=\sum_l b_{Ll}(E)\tilde{\Delta}_l(E)b_{L'l}(E), \tag{2.11}$$

so that

$$t^S_{LL'}(p',p;E)=\sum_l \tilde{t}_{Ll}(p',k;E)\tilde{\Delta}_l(E)\tilde{t}_{L'l}(p,k;E), \tag{2.12}$$

where, with $\tilde{\Delta}_l(E)$ a diagonal 2×2 matrix,

$$\tilde{t}_{LL'}(p',k;E)=\sum_l W_{Ll}(p',k;E)b_{lL'}(E). \tag{2.13}$$

If one retains only the first term on the right-hand side of Eq. (2.7) and neglects the remainder $X^{(0)}_{LL'}$, a separable representation of rank 1 for uncoupled channels and of rank 2 for the coupled channels is obtained, both having the nice feature of being exact on and half off the energy shell. Fully off shell the real quantity $X^{(0)}_{LL'}$ is in fact the corresponding absolute error.

In the following we will make use of the interesting property that the remainder $X^{(0)}_{LL'}(p',p;E)$ may be expressed in the same form (2.10) whether in terms of the W, t, and K solutions. Therefore besides Eq. (2.10), we can also write two other relations for the same $X^{(0)}_{LL'}$, namely

$$\begin{aligned}X^{(0)}_{LL'}(p',p;E) = {} & t_{LL'}(p',p;E)\\ & -\sum_{ll'} t_{Ll}(p',k;E)\\ & \times\left\{\mathbf{t}^{-1}(k,k;E)\right\}_{ll'} t_{l'L'}(k,p;E),\end{aligned} \tag{2.14}$$

$$\begin{aligned}X^{(0)}_{LL'}(p',p;E) = {} & K_{LL'}(p',p;E)\\ & -\sum_{ll'} K_{Ll}(p',k;E)\\ & \times\left\{\mathbf{K}^{-1}(k,k;E)\right\}_{ll'} K_{l'L'}(k,p;E).\end{aligned} \tag{2.15}$$

Equation (2.14) can be easily obtained by noting that $X^{(0)}_{LL'}=t_{LL'}-t^{(S)}_{LL'}$, and by using Eq. (2.4) in Eq. (2.8). One can verify the equivalence between Eqs. (2.14) and (2.15) by the use of the Heitler relation

$$\begin{aligned}t_{LL'}(p',p;E) = {} & K_{LL'}(p',p;E)\\ & -ik\frac{\pi}{2}\sum_l K_{Ll}(p',k;E)t_{lL'}(k,p;E).\end{aligned} \tag{2.16}$$

Starting from the separable representation of the t matrix t^S, one may also determine the corresponding potential that has t^S as an exact solution of the Lippmann-Schwinger equation. The resulting potential has a separable (rank 2 in the coupled-channel case) and energy-dependent form. It has the form

$$V^S_{LL'}(p',p;E) = \sum_{ll'} W_{Ll}(p',k;E)\Lambda_{ll'}(E)W_{L'l'}(p,k;E), \tag{2.17}$$

where

$$\{\mathbf{\Lambda}^{-1}(E)\}_{ll'} = \{\mathbf{\Delta}^{-1}(E)\}_{ll'} + \sum_l \int_0^\infty \frac{q^2dq}{(E-q^2)} W_{lL}(q,k;E) \times W_{lL'}(q,k;E). \tag{2.18}$$

Half-off the energy shell the separable expansion of the t matrix is exact and reduces to Eq. (2.4). Fully off of the energy shell, however, it is an approximation that varies in quality with energy. Indeed, in proximity of any energy where the quantity $W_{LL}(k,k;E)$ [or equivalently $K_{LL}(k,k;E)$] passes through zero, the separable representation acquires a pathology. For uncoupled channels, this simply coincides with the energy at which the phase shift in the relevant NN channel is zero. In coupled channels, such a pathology occurs when the determinant of $W_{LL'}(k,k;E)$ [$K_{LL'}(k,k;E)$] passes through zero, and Eq. (2.1) specifies the appropriate circumstance in terms of the phase shifts.

For uncoupled channels, Haberzettl [21] has extended the WM to higher rank. Starting with the basic W-matrix method, he succeeded in expanding the remainder matrix as a separable term plus a new remainder. The components of that separable term can be defined by a recursion formula on the original W matrices and the process is iterative. Most important, as stressed by Haberzettl [21], the expansion method conserves the reality of the successive remainder matrices and ensures that they all vanish identically half off of the energy shell on an order by order basis. Furthermore, the representation allows avoidance of a pathology (at one order below) since [21] "the potentially dangerous denominator has been modified." The procedure, in coupled channels form, is to define the (now rank 2) potentials, W matrices, and separable representations of the potential and t matrices as the zeroth order quantities $V^{(0)}_{LL'}(p',p)$, $W^{(0)}_{LL'}(p',p;E)$, $V^{S(0)}_{LL'}(p',p;E)$, and $t^{S(0)}_{LL'}(p',p;E)$, respectively. Once the quantity $V^{S(0)}_{LL'}(p',p;E)$ is determined via Eq. (2.17), the first order potential is defined to be the difference between the original input interaction, $V^{(0)}_{LL'}(p',p)$, and the zeroth order separable interaction

$$V^{(1)}_{LL'}(p',p;E) = V^{(0)}_{LL'}(p',p) - V^{S(0)}_{LL'}(p',p;E). \tag{2.19}$$

When this first order potential is used as input to the original W-matrix equation Eq. (2.3), first order W matrices result as the solutions of

$$W^{(1)}_{LL'}(p',p;E) = V^{(1)}_{LL'}(p',p;E) + \sum_l \int_0^\infty \frac{q^2dq}{(E-q^2)} \left\{ V^{(1)}_{Ll}(p',q;E) - V^{(1)}_{Ll}(p',k;E) \right\} \times W^{(1)}_{lL'}(q,p;E). \tag{2.20}$$

Their use in Eq.(2.5) gives first order Jost functions $F^{(1)}_{LL'}(E)$, in terms of which the t matrices are specified.

The procedure generalizes to any rank (i) with separation achieved if we can specify $X^{(i)}$ in terms of $X^{(i-1)}$. We have found that by extending the HM prescription [21] to coupled channels,

$$X^{(0)}_{LL'}(p',p;E) = t^{S(1)}_{LL'}(p',p;E) + X^{(1)}_{LL'}(p',p;E)\ , \tag{2.21}$$

where $t^{S(1)}$ is of separable form. Thus we define it as

$$t^{S(1)}_{LL'}(p',p;E) = \sum_{ll'} D^{(1)}_{Ll}(p',k;E)\tau^{(1)}_{ll'}(E)D^{(1)}_{L'l'}(p,k;E), \tag{2.22}$$

where

$$D^{(1)}_{L'l'}(p,k;E) = \sum_l \left[W^{(0)}_{Ll}(p',k;E) \left\{ \mathbf{W}^{(0)-1}(k,k;E) \right\}_{lL'} - W^{(1)}_{Ll}(p',k;E) \left\{ \mathbf{W}^{(1)-1}(k,k;E) \right\}_{lL'} \right] \tag{2.23}$$

and

$$\tau^{(1)}_{LL'} = \sum_{ll'} \left[\delta_{Ll} - \left\{ \mathbf{d}^{(1)-1}(E) \right\}_{Ll} \right] W^{(1)}_{ll'}(k,k;E) \left\{ \mathbf{F}^{(1)-1}(E) \right\}_{l'L'}\ , \tag{2.24}$$

where

$$d^{(1)}_{LL'}(E) = \delta_{LL'} - \sum_{ll'l''} W^{(0)}_{lL}(k,k;E) \left\{ \mathbf{F}^{(0)-1}(E) \right\}_{ll'} F^{(1)}_{l'l''}(E) \left\{ \mathbf{W}^{(1)-1}(k,k;E) \right\}_{l''L'}\ . \tag{2.25}$$

With the prescriptions of Eqs. (2.23) and (2.24), we have not reinserted a pathological condition with the inverse of the zeroth order on-shell W matrix, as the contribution then is offset by a term in the lower-rank contribution to the t matrix. But there is now the possibility of a pathology if the first order on-shell W matrix passes through zero.

In the sum then, the rank-N ($2N$ for coupled channels) separable expansions of the t matrices are given by

$$t_{LL'}(p',p;E) = \sum_{ll'} W^{(0)}_{Ll}(p',k;E)\Delta^{(0)}_{ll'}(E)W^{(0)}_{L'l'}(p,k;E) + \sum_{i=1}^{N-1}\sum_{ll'} D^{(i)}_{Ll}(p',k;E)\tau^{(i)}_{ll'}(E)D^{(i)}_{L'l'}(p,k;E) + X^{(N)}_{LL'}(p',p;E), \quad (2.26)$$

where again, the summations can be simplified if we diagonalize Δ and τ.

Clearly all first order quantities are now of rank 2 for uncoupled and rank 4 for coupled channels and they are defined once the zeroth order matrices are known.

The rank-N separable t matrix is then such that the real rank-N remainder is

$$X^{(N)}_{LL'}(p',p;E) = t_{LL'}(p',p;E) - t^{S(N)}_{LL'}(p',p;E), \quad (2.27)$$

and it is convenient to specify a correction factor by

$$C^{(N)}_{LL'}(p',p;E) \equiv \frac{|X^{(N)}_{LL'}(p',p;E)|}{|t_{LL'}(p',p;E)|}. \quad (2.28)$$

III. STURMIAN SPLITTING IN THE W-MATRIX EXPANSION

Sturmians, or equivalently Weinberg states [31], are solutions of a Schrödinger-like equation in which the energy is a continuous parameter in the range $-\infty$ to $+\infty$, and the role of spectral variable is assumed by the strength of the potential. For the NN system, the Sturmians of interest are solutions for each JST channel of

$$\frac{1}{(E-p^2)}\sum_l \int_0^\infty V_{Ll}(p,q)\phi_{l,s}(q;E)q^2dq = \eta_s(E)\phi_{L,s}(p;E). \quad (3.1)$$

In coordinate space these functions have bound-state-like boundary conditions for $E<0$, while for positive energies these functions are unnormalizable scattering states. For scattering energies, Sturmians usually (but not necessarily) have outgoing boundary conditions. If this is the case, in momentum space the singularity in $\phi_{L,s}(p,E)$ [see Eq. (3.1)] has to be eventually integrated over with the $E+i\epsilon$ prescription.

With the label s denoting a specific element of the Sturmian expansion, these states form an orthogonal set in the sense that

$$\sum_{LL'}\int_0^\infty q^2dq\int_0^\infty q'^2dq'\phi_{L,s}(q;E) \times V_{LL'}(q,q')\phi_{L',s'}(q';E) = -\eta_s(E)\delta_{ss'}, \quad (3.2)$$

where the above equations specify also the normalization that is assumed throughout the paper.

A particularly important result from the Sturmian expansion theory is that, starting from the states $\phi_{L,s}(p,E)$, we can define a set of functions

$$\chi_{L,s}(p';E) = \sum_l \int_0^\infty q^2dqV_{Ll}(p',q)\phi_{l,s}(q;E), \quad (3.3)$$

which allow the following energy-dependent expansion of the interaction

$$V_{LL'}(p',p) = -\sum_{s=1}^\infty \chi_{L,s}(p';E)\frac{1}{\eta_s(E)}\chi_{L',s}(p;E). \quad (3.4)$$

Solutions of Eq. (3.1) for positive energy are complicated by virtue of the singularity in the propagator and it is convenient to transform Eq. (3.1) into a generalized eigenvalue problem [30]. By using a damping term to Eq. (3.1) so that we have

$$\sum_l\int_0^\infty q^2dqU_{Ll}(p,q)\phi_{l,s}(q;E) = \eta_s(E)\sum_l\int_0^\infty q^2dq\,V_{Ll}(p,q)\phi_{l,s}(q;E), \quad (3.5)$$

where

$$U_{LL'}(p,p';E) = \sum_l\int_0^\infty \frac{q^2dq}{(E+i\epsilon-q^2)}V_{Ll}(p,q)V_{lL'}(q,p'), \quad (3.6)$$

the singularity problem can be overcome before the Sturmian states are found.

It may also be convenient to use Eq. (3.5) to calculate Sturmians if one wants boundary conditions that differ from the usual outgoing type. Indeed we have obtained stationary type Sturmians by retaining only the principal value integral in the expression Eq. (3.6). With normalization as given by Eq. (3.2), these principal value Sturmians [32] are then real and relevant to the specification of the K matrices that we use in the Heitler equation, Eq. (2.16), to give the complete set of t matrices.

To distinguish the stationary Sturmians from the outgoing ones, we specify them with a superscript (P). Then the K matrices are

$$K_{LL'}(p',p) = -\sum_{s=1}^\infty \chi^{(P)}_{L,s}(p';E)\left\{\frac{1}{\eta^{(P)}_s(E)[1-\eta^{(P)}_s(E)]}\right\} \times\chi^{(P)}_{L',s}(p;E) \quad (3.7)$$

effecting a separable expansion in momentum space.

In practice no more than 20 uncoupled and 40 coupled eigenvalues have to be considered in order to obtain the

expansion of the K matrices as specified by Eq. (3.7).

It is now possible to group these Sturmian expansions in such a way that the representation, which remains exact half off the energy shell, avoids the fully off-shell singular behavior of the original W-matrix method arising under the condition of Eq. (2.1) (or equivalently the $\delta = 0°$ condition in the uncoupled channels). That singularity condition Eq. (2.1) corresponds to a zero of the determinant of the on-shell K matrix $K_{LL'}(k,k;E)$ and, by virtue of Eq. (2.15), the generalized remainder acquires an off-shell pathology. To avoid this, we start with the representation given by Eq. (3.7) and split the exact K matrix as

$$K_{LL'}(p',p;E) = K^{+}_{LL'}(p',p;E) + K^{-}_{LL'}(p',p;E). \tag{3.8}$$

The matrix K^{+} is defined as

$$K^{+}_{LL'}(p',p) = -\sum_{s\in\{+\}} \chi^{(P)}_{L,s}(p';E)\left\{\frac{1}{\eta^{(P)}_s(E)[1-\eta^{(P)}_s(E)]}\right\} \times \chi^{(P)}_{L',s}(p;E) \tag{3.9}$$

within the subspace

$$s \in \{+\} \text{ if } \left[\eta^{(P)}(E)[1-\eta^{(P)}(E)]\right] > 0. \tag{3.10}$$

The matrix K^{-} is then represented in a similar manner, containing the remaining Sturmian elements, $s \in \{-\}$ *if* $\left[\eta^{(P)}(E)[1-\eta^{(P)}(E)]\right] \leq 0$. These component K matrices, K^{+} and K^{-}, are the exact reactance matrix solutions with the potentials V^{+} and $V^{-} = (V - V^{+})$, with

$$V^{+}_{LL'}(p',p;E) = -\sum_{s\in\{+\}} \chi^{(P)}_{L,s}(p';E)\frac{1}{\eta^{(P)}_s(E)}\chi^{(P)}_{L',s}(p;E), \tag{3.11}$$

and the additivity of the two K matrices is a special case of the Gell-Mann–Goldberger two potential formula [30].

We may now apply the WM separately to both the terms K^{+} and K^{-}, thereby obtaining a separable representation for each term $K^{(S)+}$ and $K^{(S)-}$ and two associated remainders $X^{(0)+}$ and $X^{(0)-}$, where

$$X^{(0)+}_{LL'}(p',p;E) = K^{+}_{LL'}(p',p;E) - \sum_{ll'} K^{+}_{Ll}(p',k;E)\left\{\mathbf{K}^{+^{-1}}(k,k;E)\right\}_{ll'} K^{+}_{l'L'}(k,p;E), \tag{3.12}$$

and similarly for $X^{(0)-}$.

Now $\det(\mathbf{K}^{+})$ may be written as

$$\det(\mathbf{K}^{+}) = \sum_{i,j\in\{+\}} \chi^{(P)}_{0i}\chi^{(P)}_{2j}\frac{\chi^{(P)}_{0i}\chi^{(P)}_{2j} - \chi^{(P)}_{2i}\chi^{(P)}_{0j}}{\eta^{(P)}_i\eta^{(P)}_j(1-\eta^{(P)}_i)(1-\eta^{(P)}_i)} = \frac{1}{2}\sum_{i,j\in\{+\}} \frac{[\chi^{(P)}_{0i}\chi^{(P)}_{2j} - \chi^{(P)}_{2i}\chi^{(P)}_{0j}]^2}{\eta^{(P)}_i\eta^{(P)}_j(1-\eta^{(P)}_i)(1-\eta^{(P)}_j)}, \tag{3.13}$$

where $\chi^{(P)}_{Li}[\equiv \chi^{(P)}_{Li}(k,E)]$ is the on-shell form factor. Since both summation indices in Eq. (3.13) span the subspace $\{+\}$, and the stationary states in the numerator are all normalized as real functions, all the elements in the summation are positive. This is always true if the stationary Sturmian eigenvalues are all real. For positive energy however, complex conjugated pairs (CCP) may occur; bringing into question the use of the method. But we find that if such CCP's are coupled correctly, their summation in determining the reactance matrices may be always recast into a form which involves purely real quantities, since all the imaginary components cancel [33].

Further since the elements (of K^{+}) are all positive, the determinant is non-null, unless all the elements of the summation are individually zero. The same reasoning applies with $\det(\mathbf{K}^{-})$. If we assume at least three states in both subspaces (otherwise K^{+}, or K^{-}, or both, are already of rank 2 or less and this SSM is inappropriate), a zero in the determinants occur only if the ratios

$$R_i = \frac{\chi^{(P)}_{2i}}{\chi^{(P)}_{0i}}, \tag{3.14}$$

are independent with respect to i belonging to a specific subset ($\{+\}$ or $\{-\}$). Although, in principle, we cannot exclude this extreme situation, realistic NN interactions have a local component and, therefore, the number of Sturmians is infinite. Therefore, if we use a suitable large number of Sturmians as a basis set, the problem of the independence of R_i may be resolved.

Thus, we may use the Sturmian splitting method to separate the K matrix into two pieces K^{+} and K^{-}, both of which are amenable to a W-matrix representation. The ensuing t matrix is free of any pathology arising fully off shell when $\det(\mathbf{K})$ vanishes. Finally, the total K matrix can be approximated in a separable form $K^{(S)}$,

$$K^{(S)}_{LL'}(p',p;E) \equiv K^{(S)+}_{LL'}(p',p;E) + K^{(S)-}_{LL'}(p',p;E), \tag{3.15}$$

with a global error given by

$$X^{(0)}_{LL'}(p',p;E) = X^{(0)+}_{LL'}(p',p;E) + X^{(0)-}_{LL'}(p',p;E). \tag{3.16}$$

This representation, which is exact on and half off the

energy shell, is specified when $K^{(S)\pm}$ is obtained through the type of representation given by Eq. (2.12). But these must refer to potentials, $V^{\pm}$, defined via Eq. (3.11). Each partial reactance matrix, $K^{(S)\pm}$, may also be recast in the form

$$K^{(S)\pm}_{LL'}(p',p;E) = \sum_{ll'} K^{\pm}_{Ll}(p',k;E)\left\{\mathbf{K}^{\pm\,-1}(k,k;E)\right\}_{ll'} \times K^{\pm}_{l'L'}(k,p;E), \tag{3.17}$$

which exhibits the regularity of the representation since $K^{\pm}_{LL'}$, on shell, are always invertible even if their sum, $K_{LL'}$, is not. Finally, from the separable approximation for the K matrix, one can obtain (via the Heitler equation) a representation of same rank for the t matrix. Also, because of the half-off-shell exactness of the approximation, Eq. (3.16) also represents the error with this separable representation of the t matrix.

This Sturmian split representation has all the advantages of the original WM scheme. It gives an exact representation for both the K and t matrices half off of the energy shell, with the imaginary component of the t matrix being exact also fully off shell. With respect to the original WM scheme, the Sturmian split W matrix representation avoids pathologies that exist in the original WM representation.

IV. RESULTS

To investigate the accuracy of the HM, SSM, and WM separable representations of t matrices, we have calculated the correction factors for each. Those factors are displayed as contour plots, with the contour lines giving differences between exact and a given separable result of 5%, 10%, 15%, and 25%. We use the Paris interaction [11] in the Lippmann-Schwinger equations to generate the exact t matrices for each method.

The correction factors $C_{LL'}$ for the singlet $^1S_0$ channel are displayed in Figs. 1–3. The on-shell point is given by the dots in each panel. Clearly, in all cases, the correction factor is zero half off shell. Those correction factors obtained using the original, rank-1 WM [18] have been displayed previously (Fig. 2 of Ref. [20]) while those obtained with the rank-2 HM formalism [21] at six energies are shown here as Fig. 1. It is evident from Ref. [20] that the original WM gives a very good description of the exact t matrices for energies up to 100 MeV. Also comparison with the corresponding results for $E < 100$ MeV in Fig. 1, show that generally they are better than the factors obtained using the rank-2 HM. This is due to the occurrence of a new pathology within the $^1S_0$ channel at first order (rank 2). At 9 MeV, the on-shell rank-2 W matrices $[W^{(1)}_{LL}(k,k;E)]$ pass through zero for the Paris interaction, so creating a new pathology. At higher rank, this new pathology disappears. It is found that this rank-2 pathology is interaction dependent, occurring also for the BonnQ [12] but not for the Reid interaction [29]. Therefore since one cannot exclude the possible occurrence of new pathologies when dealing with realistic nucleon-nucleon potentials, the method proposed in Ref. [21] (HM) seems to have some serious limitations.

The $^1S_0$ phase shift passes through zero at an energy of about 232 MeV, and consequently the off-shell description given by the original WM scheme becomes quite inadequate [30]. Around this energy, the modified HM avoids the zero-phase pathology, and so improves the fully-off-shell description of the t matrices.

Although we are mainly interested in *low*-rank separable approximations, nevertheless we studied for completeness the HM behavior at higher orders. The results displayed in Fig. 2 were obtained for the $^1S_0$ channel at 200 MeV. From this it is evident that the HM separable approximation to the exact t matrix improves with rank. However, the improvements obtained going from zeroth to second order (namely, from rank 1 to rank 3) are not impressive, but, by increasing one order further, the result improves markedly. Indeed, the rank-4 result gives an excellent description of the exact t matrix at 200 MeV, while the representations with rank higher than 6 are practically indistinguishable from the exact t matrices.

In Fig. 3, we show the results obtained using the SSM (rank 2) for the $^1S_0$ channel. Comparisons with the results given in Fig. 1 and those of Ref. [20] again show that, for energies below 100 MeV, the original WM still gives the best description, although the results of the SSM are only slightly inferior. At energies above 100 MeV the SSM has better accuracy than the other prescriptions. At 150 MeV, it should be noted, the large percentage error for momenta above the on-shell value

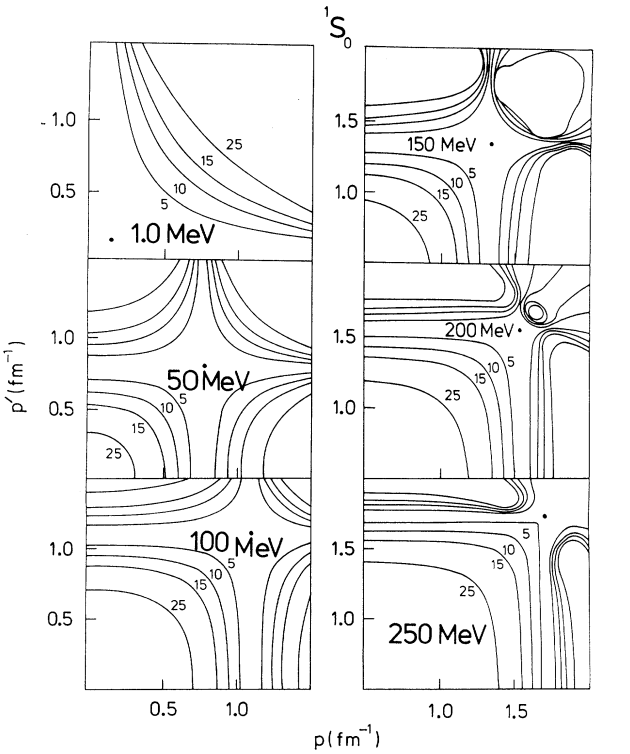

FIG. 1. Contour plots of the correction factor to the rank-2 W-matrix separable approximation of Haberzettl for the (Paris interaction) $^1S_0$ t matrices at a variety of lab energies. The contours shown are 5%, 10%, 15%, and 25%.

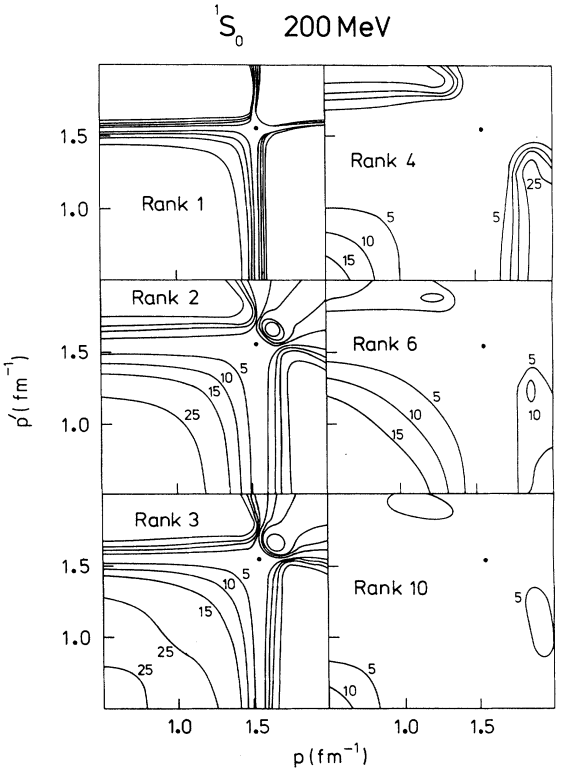

FIG. 2. Contour plots of the correction factor to the separable approximation for the Haberzettl method at ranks 1, 2, 3, 4, 6, and 10 for the (Paris interaction) $^1S_0$ t matrices at a lab energy of 200 MeV.

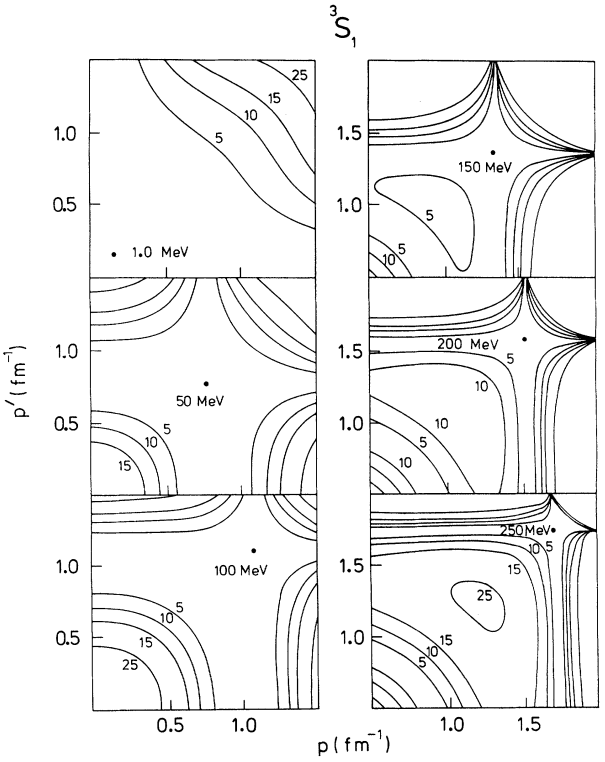

FIG. 4. Same as Fig. 1 but for the rank-4 W-matrix separable approximation of Haberzettl for the $^3S_1$ channel.

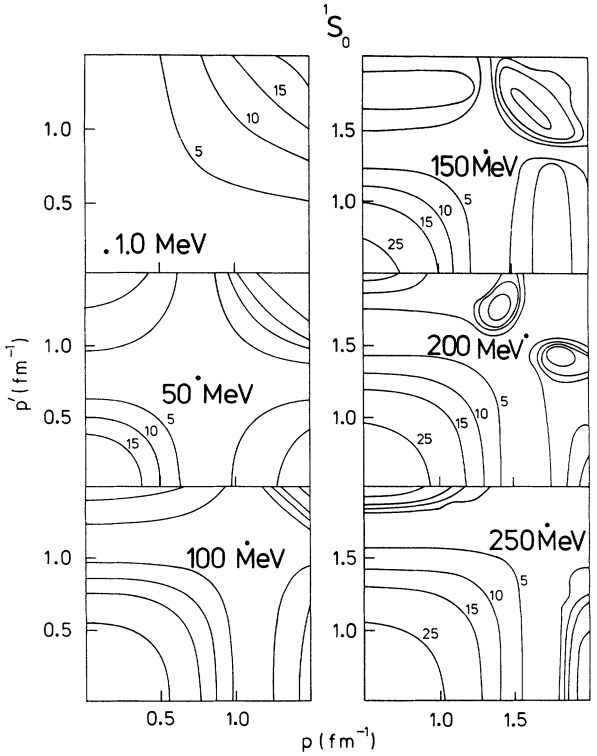

FIG. 3. Same as Fig. 1 but for the SSM separable approximation of rank 2.

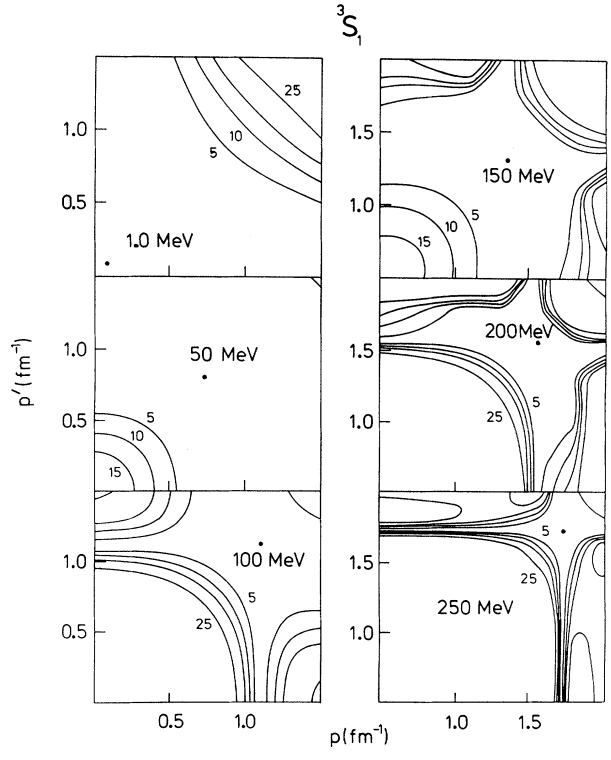

FIG. 5. Same as Fig. 4 but for the SSM separable approximation of rank 4.

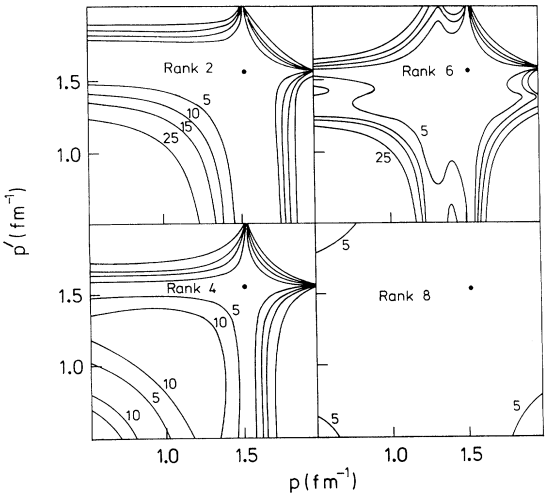

FIG. 6. Contour plots of the correction factor to the separable approximation for the Haberzettl method at ranks 2, 4, 6, and 8 for the (Paris interaction) $^3S_1$ t matrices at a lab energy of 200 MeV.

is really an anomaly with the correction factors. In this region, the full off-shell t matrices become small (approximately 1% of the on-shell results), with the real component of the t matrices passing through zero. Therefore the denominator in Eq. (2.28) is small in this region. Thus, even though the differences between the exact and separable representation values are very small, any such difference is magnified greatly by the ratio. This is not unlike the problem encountered by others [34] when comparing K and t matrices and using the Kowalski–Noyes f ratios [24, 35]. The results between 200 and 250 MeV reveal that the SSM gives a much better approximation to the $^1S_0$ t matrices than the method of Ref. [21] (Fig. 1).

The $^3S_1$ WM (Fig. 5, Ref. [20]) and HM (Fig. 4, this work) results are compared with the equivalent, rank-4, SSM calculations shown in Fig. 5. The result of the comparison of the three methods in the $^3S_1$ channel is more complex than those of the $^1S_0$ channel. In the range 1:100 MeV both HM and SSM improve the WM results. Around 1 MeV, HM and SSM are similar, at 50 MeV the SSM has the most observable improvement, and at 100 MeV, the HM (SSM) is more accurate for lower (higher) momenta. In the range 150:250 MeV the WM and HM are similar (the WM being slightly better), while the SSM has high accuracy in a larger region centered on the on-shell point, but the SSM accuracy deteriorates much faster going far from the on-shell point, especially for low momenta.

For completeness, we show in Fig. 6 the higher-order HM properties for the triplet channel. Here, at 200 MeV, it is seen that the original WM (rank 2) gives a better description off shell than does the corresponding rank-4 HM result at 200 MeV. However, by going to the next order (rank 6), an improvement in the comparison is readily seen. An increase of a further order (to rank 8) gives an off-shell description of the 200 MeV t matrix which is virtually exact over the momentum range considered.

V. CONCLUSION

The original WM has been shown, both here and previously [20], to give an extremely good approximation to the fully-off-shell NN t matrices and as rank-1 (uncoupled) and rank-2 (coupled) separable forms at low energies, while being exact on and half off of the energy shell. But the method is inherently flawed, in that if the phase (or on-shell determinant) pass through zero, a pathology exists.

Herein, we considered two methods, both of which are able to alleviate the problems of such pathologies. The first is the HM prescription which we have extended to coupled channels. Although it is impossible in this scheme to eliminate completely all the sources of pathologies, since a singularity occurs at any rank N when $W^{(N-1)}(k,k;E) = 0$ [for coupled channels, at any rank $2N$ when $\det\mathbf{W}^{(N-1)}(k,k;E) = 0$], our numerical study within a realistic NN force shows that with increasing rank (up to 8 for the S states) this method gives an excellent description of the exact fully-off-shell results in both coupled and uncoupled channels. If any new off-shell singularity arises at a given rank, by increasing the rank by 1 the problem may be possibly overcome. But of concern is the onset of new pathologies of this method which are interaction dependent.

The second method the SSM was based upon selective summations of components of a Sturmian expansion of the reactance matrices. The selection was made so that the attractive Sturmians (positive components in the separable expansion) and the repulsive Sturmians (negative components in the separable expansion) separate. The original W-matrix procedure was then applied independently to each term. The advantage of the method with respect to the previous ones is that *no pathology occurs* as these two separated t matrices are always nonzero on the energy shell, even when their summations produce null on-shell t matrices. This scheme leads to rank-2 (rank-4) separable approximation of the t matrices for uncoupled (coupled) channels, which nevertheless remain exact on and half off of the energy shell. The method describes remarkably well the fully-off-shell properties of the t matrices up to quite high energies (at least 250) MeV, while keeping the rank of the separation as low as possible in order to be used in three- or more-body calculations.

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