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Matrix-Shape Approach to Elastic Scattering

Robert Conn
Nuclear Engineering Department, University of Wisconsin, Madison, Wisconsin 53706

and

Herschel Rabitz*
Chemistry Department, Princeton University, Princeton, New Jersey 08540
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The theory and application of the matrix-shape (MS) approach is investigated for elastic scattering. Various aspects of the method, such as the choice of appropriate variables, the choice of basis-set functions as representations of the T matrix, and the use of a MS fit to the potential matrix that allows VG_0^+T-type integrals to be performed analytically, are considered. The method is applied to three-dimensional elastic scattering to ascertain if, on this widely studied problem, the MS approach can in fact produce the essential physics. Numerical calculations are presented to illustrate that reasonable results can be achieved. The numerical results were obtained using two special cases of the method of weighted residuals, which can be used with the MS approach to solve the Lippmann–Schwinger equation for T. The use of the MS approach in conjunction with variational principles is also discussed.

I. INTRODUCTION

Many experimental data on scattering processes involving large numbers of open channels have become available in the last few years[1] and many approximate methods[1–3] are being studied for application in this area. For most of these problems, the coupling between channels is strong enough that methods based on the Born approximation and modifications thereto do not work.[4] Close-coupling methods have been developed[5] but they remain expensive and limited to the order of 100 open channels. Yet even in simple scattering problems, large numbers of coupled channels can be involved. It is also true that the experimental results generally involve averages over the many states involved and the need for exact state-to-state transition probabilities is perhaps questionable in very large problems. Approximate nonperturbative solutions to scattering problems of this type, based upon the construction of approximate transition matrices that follow the essential functional and variable dependence of the exact transition matrix, would be very useful for analysis in this area. In a recent paper,[6] such a nonperturbative approximate approach (the matrix-shape or MS approach) to scattering problems was suggested and based upon the general variable dependence or "shape" of the matrices that contain the scattering information. The applicability of this approach was indicated in a quantitative way by examination of the collinear atom-diatomic vibrationally inelastic-scattering problem.

In this paper, we expand and further develop these ideas and, as well, examine more quantitatively the viability and sensitivities of this approach. Our goal is to gain a deeper understanding of the underlying ideas and to examine the method to determine if quantitative, and physically reasonable, results can be obtained. As such, this paper deals with the use of the MS approach in three-dimensional elastic-scattering problems. We will deal further with inelastic scattering in future publications since the method, as we will develop it in Sec. II, can be extended to more difficult problems where approximate answers for transition probabilities would be highly desirable. We want here to determine if, on well-known elastic-scattering problems, the method can extract the relevant physics contained in quantities such as the total cross section and its variation with energy. Further, it will be possible to develop some experience with regard to the number of terms required in a basis-set expansion, the appropriate variables that are most important in a description of the T matrix, and whether such expansions can yield, within a few percent, the relevant scattering information. It is in this context that we shall discuss the numerical results presented in Sec. V.

II. THEORY

A. General Equations

The physical information in quantum-mechanical scattering is contained in the T matrix. The transition probabilities and scattering cross sections can be found directly once T is known. One can, of course, work in coordinate space to generate approximate wave functions and then form the matrix elements from which the physical information can be obtained. However, it is perhaps more appropriate to work directly in quantum-number space

since T is directly related to quantities of physical interest. The T matrix, with matrix elements $\langle\alpha'|T|\alpha\rangle$, satisfies the integral equation[7]

$$\langle\alpha'|T|\alpha\rangle = \langle\alpha'|V|\alpha\rangle + \int\langle\alpha'|V|\alpha''\rangle G_0^+(\alpha'', E)\langle\alpha''|T|\alpha\rangle , \quad (1)$$

where V is the interaction potential operator; $G_0^+(\alpha'', E)$ is

$$G_0^+(\alpha'', E) = \frac{1}{E - E_{\alpha''} + i\epsilon} ; \quad (2)$$

and $|\alpha\rangle$ is an eigenstate of the unperturbed Hamiltonian H_0,

$$H_0|\alpha\rangle = E_\alpha|\alpha\rangle , \quad (3)$$

with E the total energy in the center-of-mass system. Equation (1) is the well-known Lippmann–Schwinger (LS) equation[7] for the transition matrix T. For elastic scattering, the LS equation for the T matrix is Eq. (1), identifying α with the wave vector $\vec{k}$ and α' with $\vec{k}'$.

For future reference, the differential-scattering cross section is related to the T matrix via

$$\frac{d\sigma}{d\Omega} = \frac{(2\pi)^4\mu^2}{\hbar^4}\,|\langle\vec{k}'|T|\vec{k}\rangle|^2 , \quad (4)$$

where μ is the reduced mass. The total cross section σ_T^{int} is obtained by integrating $d\sigma/d\Omega$. Additionally, one can use the optical theorem[7] to obtain the total cross section σ_T from the imaginary part of the on-shell T matrix in the forward direction:

$$\sigma_T^{\text{op}} = -(16\pi^3\mu/\hbar^2 k)\,\text{Im}(\langle\vec{k}'|T|\vec{k}\rangle)_{\vec{k}'=\vec{k}} . \quad (5)$$

This is just a statement of unitarity and, for the exact T matrix, $\sigma_T^{\text{int}} = \sigma_T^{\text{op}}$. However, approximate T matrices will not automatically yield unitary results, and a comparison of σ_T^{int} and σ_T^{op} can provide a measure of the accuracy of T.

B. Characteristic Variables and Expansion of T Matrix

The approximate nonperturbative method we are developing is based on the idea of expanding the relevant matrices in functions that follow the main variable dependencies of these matrices.[6] To see more clearly the ideas involved, consider elastic scattering from a three-dimensional spherically symmetric potential. In this case,[8] the V matrix elements $\langle\vec{k}'|V|\vec{k}\rangle$ depend upon $(\vec{k}'-\vec{k})^2$ and not, for example, on $\vec{k}'$ and $\vec{k}$ separately or in other forms such as $\vec{k}'+\vec{k}$. It is clear then that an expansion of V in functions dependent upon $(\vec{k}'-\vec{k})^2$ can most readily follow the main variable dependence of V. It would in general be considerably more difficult to represent the V matrix by using an expansion in a sum of products of functions[9] depending separately on $\vec{k}'$ and $\vec{k}$, such as

$$\langle\vec{k}'|V|\vec{k}\rangle \simeq \sum f_i(\vec{k}')g_i(\vec{k}) . \quad (6)$$

It has been shown[10–12] that in the high-energy limit the major variable dependence of T is also on $(\vec{k}-\vec{k}')^2$. Thus, one major variable dependence of T in three-dimensional elastic scattering should be on the difference variable

$$\kappa^2 = (\vec{k}'-\vec{k})^2 . \quad (7)$$

However, it is clear that away from the high-energy limit, κ^2 cannot be the sole variable dependence of T. The sum variable $s^2 = (\vec{k}+\vec{k}')^2$ $[\vec{s} = (\vec{k}+\vec{k}')]$ is conjugate to κ^2, and each will dominant in a separate hemisphere corresponding to the forward and backward directions, on shell. A third variable is required for a complete description of T off shell, and a natural choice in light of the above discussion is the dot-product variable $\vec{\kappa}\cdot\vec{s}$. We expect, however, that the on-shell range of T is most important physically and, since $\vec{\kappa}\cdot\vec{s} = 0$ on shell, this variable is likely to be less important than κ^2 and s^2. In summary, the "characteristic variable" choices are

$$v^2 = (\vec{k}'-\vec{k})^2 A_0^2 , \quad (8)$$

$$u^2 = (\vec{k}+\vec{k}')^2 A_0^2 , \quad (9)$$

$$w = \vec{u}\cdot\vec{v} , \quad (10)$$

where the factor A_0 in Eqs. (8) and (9) is the characteristic length in the problem (such as the range of the potential).

The choice of variables such as v^2 and u^2 to describe the main variable dependence of the T matrix has been noted several times in the literature[7,13,14] and they have been widely used in dispersion theory to extract information on the behavior of the T matrix.[7] The MS approach is based on a direct use of these variables. Also, we note that our choice of variables (and the expansion functions to be discussed) is not based upon a unitary transformation on T. The efforts made to choose characteristic variables are physically motivated and are analogous to looking for the normal coordinates of the problem which, unfortunately, remain unknown.

C. Scattering Potential: MS Fit

In this paper we examine potentials of the general form[15]

$$V(r) = -V_0\int_0^\infty dx\, A(x)e^{-xr^2} . \quad (11)$$

Many of the standard potentials; such as the Gaussian, Yukawa, and exponential, are of this form.[16] A primary reason for using the form in Eq. (11) is that we have been able to carry out the integrals over the intermediate states in the LS equation (1) analytically. With Eq. (11), the V matrix becomes

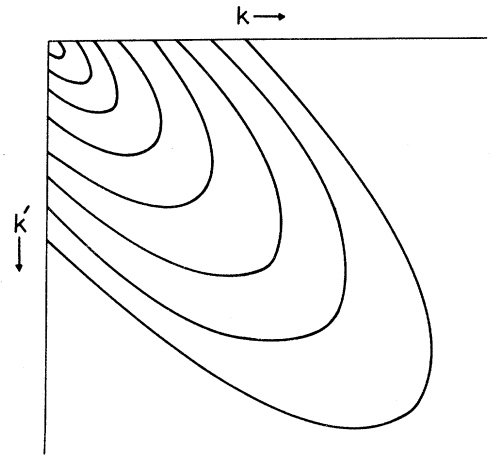

FIG. 1. Schematic diagram illustrating the shape of the V matrix. The diagonal elements $(k=k')$ dominate and the elements decay in magnitude as $(k-k')$ increases.

$$\langle \vec{k}' | V | \vec{k} \rangle = \frac{-V_0}{8\pi^{3/2}} \int_0^\infty dx \frac{A(x) e^{-(\vec{k}-\vec{k}')^2/4x}}{x^{3/2}} \quad . \tag{12}$$

In the numerical computations to be presented, we have given particular attention to the Yukawa potential

$$V(r) = (-V_0 A_0/r) e^{-r/A_0} \quad , \tag{13}$$

since it has been widely studied in the literature.[17-20] For this potential the function $A(x)$ is

$$A(x) = [1/(\pi x)^{1/2}] e^{-1/4A_0^2 x} . \tag{14}$$

Equation (12) yields the well-known result

$$\langle \vec{k}' | V | \vec{k} \rangle = \frac{-V_0 A_0^3}{2\pi^2} \frac{1}{1+v^2} \quad . \tag{15}$$

In general the integral in Eq. (12) would be performed numerically,

$$\langle \vec{k}' | V | \vec{k} \rangle \approx \frac{-V_0 A_0^3}{2\pi^2} \sum_{l=1}^{N_a} a_l e^{-t_l v^2} , \tag{16}$$

using Gauss–Laguerre weights and abscissa.[21] Equation (16) can be viewed as a MS fit to the potential matrix. It exhibits the general characteristic that it decays away for sufficiently large v. This is illustrated in Fig. 1, where scalar k and k' are used for simplicity.

III. CHOICES OF BASIS-SET EXPANSION FUNCTIONS

Two general expansions of T have been investigated, one based on expansions in Hermite polynomials and another based upon expansions in trigonometric functions. The choice of expansion functions in the MS method is based on several guiding principles. First, the T matrix is expected, as with the V matrix, to depend upon the variables we have already discussed and in a manner analogous to that illustrated for V in Fig. 1. Second, the functions must be linearly independent and hopefully complete. A third guiding idea is to choose functions with which analytical evaluations can be carried as far as possible. For example, Gaussian functions, such as $e^{-\gamma_i v^2}$, $e^{-\alpha_i u^2}$, etc., have the appropriate functional behavior and allow one to proceed in terms of analytical evaluations of integrals in the LS equation. However, expansion in Gaussian functions can lead to serious numerical difficulties because such functions are only weakly linear independent.[6]

The first general expansion used is an expansion of T in Hermite polynomials in v^2 and u^2, multiplied by Gaussian weight factors. These functions will retain the basic MS approximation to T while adding to the numerical stability of the problem. Furthermore, as we will show, the integrals in the LS equation can be worked analytically.

We have expanded using only u^2 and v^2 for reasons previously discussed, namely, that the on-shell range of T is the most important for the solution of the LS equation in many scattering problems.[10,11] This approach therefore amounts to an effort to synthesize T from functions of v^2 and u^2 by finding appropriate expansion coefficients. The expansion itself, labeled H-1, is

$$\langle \vec{k}' | T | \vec{k} \rangle \simeq \left(\sum_{i=0}^{N_v} x_i \psi_i(v) + \sum_{i=1}^{N_u} y_i \phi_i(u) \right) \left(\frac{-V_0 A_0^3}{2\pi^2} \right) , \tag{17}$$

where

$$\psi_i(v) = \sum_{l=1}^{N_a} a_l e^{-t_l v^2} , \qquad i = 0$$
$$= e^{-\gamma v^2} H_{2i}(v^2) , \qquad i \geq 1 \tag{18}$$
$$\phi_i(u) = e^{-\alpha u^2} H_{2i-1}(u^2) , \quad i \geq 1 \tag{19}$$

and $H_i(x)$ are the Hermite polynomials.[22] This structure requires some further explanation. The leading term in v^2, $\psi_0(v)$, is the potential matrix in Eq. (16) except for numerical constants. The expansion involves even-order Hermite polynomials in v^2 and odd-order Hermites in u^2. Since both variables range only over $[0, \infty]$, both expressions are separately complete.[23] The reason for this choice is to ensure linear independence on shell because on shell, v^2 and u^2 are not independent but are related by

$$v^2 + u^2 = 4A^2 \quad \text{(on shell)} , \tag{20}$$

where $A^2 \equiv k^2 A_0^2$. The Gaussian terms $e^{-\gamma v^2}$ and $e^{-\alpha u^2}$ are included to guarantee convergence of all integrals in the problem and to provide an over-all matrix shape.

Another expansion that is really a subset of choice H-1 is an expansion in Hermites dependent solely on v^2. This set is

$$\langle \vec{k}' | T | \vec{k} \rangle \simeq \left(\sum_{i=0}^{N_v} x_i \psi_i(v) \right) \left(-\frac{V_0 A_0^3}{2\pi^2} \right) , \tag{21}$$

where, now, $\psi_i(v)$ is defined by

$$\psi_i(v) = \sum_{l=1}^{N_a} a_l e^{-v^2 t_l} , \quad i = 0$$

$$= e^{-\gamma v^2} H_i(v^2), \quad i \geq 1 . \tag{22}$$

Since only v^2 enters as a variable, all the Hermites in v^2 can be used. This choice, labeled H-2, allows us to examine the behavior of the results on the variable dependence.

At this point, a disclaimer is in order regarding the completeness of the expansion functions in the space of T. While it is true that the functions in (18) and (19) are separately complete on $[0, \infty]$, these expansions do not span the complete (u^2, v^2, w) space of T. We argue simply that the functions span v^2 and u^2 individually and, based on the previous discussion, they are expected to span that part of the space of T most important for the physics of the problem. Certainly, they span the on-shell range and to the extent that this range is most important, our expansion will give adequate results. The reasonableness of the numerical results bears out this point.

The second general basis set examined is an expansion of T in sines and cosines complete over a multiple of the on-shell range. Unlike the Hermites, which are complete on the semi-infinite interval $[0, \infty]$ (and therefore can perhaps better represent T off shell), the sine-cosine expansion set will be complete in u^2 and v^2 only over a finite interval. Again, the motivation for examining this choice is the many indications that the on-shell range is physically most important. (Certainly, to the extent that classical mechanics is correct, this is true.) Thus, the expansion in sines and cosines, labeled SC-1, is of the same form as Eq. (17) but with $\psi_i(v)$ and $\phi_i(u)$ now defined as

$$\psi_i(v) = \sum_{l=1}^{N_a} a_l e^{-v^2 t_l} , \qquad i = 0$$

$$= e^{-\gamma v^2} \cos(\omega_i v^2) , \quad i \geq 1 \tag{23}$$

$$\phi_i(u) = e^{-\alpha u^2} \sin(\omega_i u^2) , \quad i \geq 1 . \tag{24}$$

As before, $\psi_0(v)$ is given by Eq. (16). The frequencies ω_i are defined by

$$\omega_i = (i/M_0)\omega_0 , \tag{25}$$

$$\omega_0 = \pi/2A^2 , \tag{26}$$

where $[0, 4A^2]$ is the on-shell range of u^2 and v^2, separately. Choosing different values of M_0 implies using a fundamental frequency related to a multiple of the on-shell range. We have found $M_0 = 2$ to give satisfactory results. The expansion functions remain, as with the Hermites, linearly independent on shell. An additional advantage to using sines and cosines is that they lead to relatively simple expressions for the intermediate-state integral in the VG_0^+T term of the LS equation (1) (see Appendix B).

IV. APPROXIMATE NONPERTURBATIVE SOLUTION OF LS EQUATION

In this section, we sketch the derivation of the equations to be solved for the expansion coefficients in the basis-set expansions of T. Some of the expressions are referred to in Appendixes A and B.

A. Galerkin Method and Hermite-Polynomial-Expansion Set

The Galerkin method[24,25] has been used to obtain a set of algebraic equations to solve for the complex expansion coefficients x_i and y_i in Eq. (17). Since Eq. (17) gives an approximation to T, when it is substituted into Eq. (1), the difference between the left- and right-hand sides defines a residual function,

$$R(u, v) = \sum_{i=0}^{N_v} x_i \psi_i(v) + \sum_{i=1}^{N_u} y_i \phi_i(u) - \psi_0(v)$$

$$- c \int d^3Q'' \left[\psi_0(v_2) \left(\sum_{i=0}^{N_v} x_i \psi_i(v_1) + \sum_{i=1}^{N_u} y_i \phi_i(u_1) \right) \Big/ \right.$$

$$\left. (A^2 - Q''^2 + i\epsilon) \right] \tag{27}$$

where $c = -(V_0/E)(A^2/2\pi^2)$, $\vec{Q}'' = \vec{k}'' A_0$, and the variables v_1, u_1, and v_2 are

$$v_1^2 = (\vec{k}'' - \vec{k})^2 A_0^2 , \tag{28}$$

$$u_1^2 = (\vec{k}'' + \vec{k})^2 A_0^2 , \tag{29}$$

$$v_2^2 = (\vec{k}' - \vec{k}'')^2 A_0^2 . \tag{30}$$

The N $(= N_u + N_v + 1)$ simultaneous linear equations for x_i and y_i are

$$\int d^3u \, d^3v \, R(u, v) \Lambda_n^{\pm}(u, v) = 0 , \tag{31}$$

where

$$\Lambda_n^{\pm} = \psi_{(n-1)/2}(v) e^{-\alpha u^2}$$

$$= \phi_{n/2}(u) e^{-\gamma v^2} ; \tag{32}$$

$+$ implies $n = 1, 3, \ldots, 2N_v + 1$, $-$ implies $n = 2, 4, \ldots, 2N_u$, and the exponential functions are included as convergence factors for the integrals. Explicitly, the equations for x_i and y_i are

$$\sum_{i=1}^{N_u} y_i W_i^{\pm}(n, i) + \sum_{i=0}^{N_v} x_i W_2^{\pm}(n, i) - W_2^{\pm}(n, 0)$$

$$- c \sum_{l=1}^{N_a} a_l \left(\sum_{i=1}^{N_u} y_i W_3^{\pm}(n, i; l) + \sum_{i=0}^{N_v} x_i W_4^{\pm}(n, i; l) \right) = 0 , \tag{33}$$

with the functions $W_m^{\pm}$ defined by

$$W_1^{\pm}(n,\ i)=\int d^3u\, d^3v\, \Lambda_n^{\pm}(u,\ v)\phi_i(u)\,, \tag{34}$$

$$W_2^{\pm}(n,\ i)=\int d^3u\, d^3v\, \Lambda_n^{\pm}(u,\ v)\psi_i(v)\,, \tag{35}$$

$$W_3^{\pm}(n,\ i;\ l)=\int d^3u\, d^3v\, d^3Q''\,\frac{\Lambda_n^{\pm}(u,\ v)\,e^{-v_2^2 t_l}\phi_i(u_1)}{A^2-Q''^2+i\epsilon}\,, \tag{36}$$

$$W_4^{\pm}(n,\ i;\ l)=\int d^3u\, d^3v\, d^3Q''\,\frac{\Lambda_n^{\pm}(u,\ v)\,e^{-v_2^2 t_l}\psi_i(v_1)}{A^2-Q''+i\epsilon}\,. \tag{37}$$

All these functions have been evaluated analytically and the derivation and final expressions are given in Appendix A. We now define a matrix

$$\underline{S}=\{S_{nj}\} \tag{38}$$

with matrix elements

$$S_{nj}=\begin{cases} W_1^{-}(n,\ \tfrac{1}{2}j)\,, & j \text{ even};\ n \text{ even} \\ W_2^{-}(n,\ \tfrac{1}{2}(j-1))\,, & j \text{ odd};\ n \text{ even} \\ W_1^{+}(n,\ \tfrac{1}{2}j)\,, & j \text{ even};\ n \text{ odd} \\ W_2^{+}(n,\ \tfrac{1}{2}(j-1))\,, & j \text{ odd};\ n \text{ odd} \end{cases} \tag{39}$$

and a matrix

$$\underline{C}=\{C_{nj}\}\,, \tag{40}$$

with matrix elements

$$C_{nj}=c\sum_{l=1}^{N_a} a_l \times \begin{cases} W_3^{-}(n,\ \tfrac{1}{2}j;\ l)\,, & j \text{ even};\ n \text{ even} \\ W_4^{-}(n,\ \tfrac{1}{2}(j-1);\ l)\,, & j \text{ odd};\ n \text{ even} \\ W_3^{+}(n,\ \tfrac{1}{2}j;\ l)\,, & j \text{ even};\ n \text{ odd} \\ W_4^{+}(n,\ \tfrac{1}{2}(j-1);\ l)\,, & j \text{ odd};\ n \text{ odd}\,. \end{cases} \tag{41}$$

Defining a solution vector of length N as

$$b=\begin{pmatrix} x_0 \\ y_1 \\ x_1 \\ y_2 \\ \vdots \end{pmatrix} \tag{42}$$

and the vector a as

$$a=\begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix} \tag{43}$$

the matrix equation to be solved for b is

$$(\underline{S}-\underline{C})\,b=\underline{S}\,a\,, \tag{44}$$

where $\underline{S}$ and $\underline{C}$ are $(N_u+N_v+1)\times(N_v+N_v+1)$ complex matrices.

B. Collocation Method and Sine-Cosine Basis Set

The collocation method[24] has been used to obtain the expansion coefficients in the sine-cosine basis set. The equations for these coefficients are obtained by considering the residual function $R(u, v)$, as defined by Eq. (27), using Eqs. (23) and (24) as the definitions of $\psi_i(v)$ and $\phi_i(u)$, respectively.

To employ collocation, one must set the residual equal to zero at $N_v+N_u+1\equiv N$ collocation points to obtain the required number of equations. Since the on-shell range is most important, the collocation points will be chosen within this range. Furthermore, since $u^2=4A^2-v^2$ on shell, one in practice chooses N collocation values of v^2. In addition, the values of the collocation points on shell are chosen to be the zeros of the shifted Chebychev polynomials[26] of order N. The reason for this choice is that $T_N^*(x)$, the shifted Chebychev polynomial on $[0,\ 1]$ of order N, has equal magnitude extrema.[27] If $T_N^*(x)$ is considered the error curve resulting from an attempt to obtain a best fit to x^n on $[0,\ 1]$ using a polynomial of order $N-1$, then this error curve will exhibit "equal ripples"[27] (it is a "normal" error curve). We would like to choose the collocation points v_j^2 such that the residual function $R(v^2)$ on shell has equal magnitude extreme deviations from zero and that these deviations are as small as possible. Of course, when $R(v^2)$ is computed, it may not have the "equal-ripple" property, but the choice of collocation points as zeros of the shifted Chebychev polynomial nevertheless represents a most reasonable first guess.[27] Therefore, the collocation points are

$$v_j^2=4Q^2\cos^2\left(\frac{2j-1}{4N}\,\pi\right)\,. \tag{45}$$

It is interesting to note that for $N=1$ the value of v_j^2 corresponds to $\theta=\frac{1}{2}\pi$ (θ is the center-of-mass scattering angle). One can readily show that in this case x_0 is

$$x_0=f_1(\tfrac{1}{2}\pi)/[\,f_1(\tfrac{1}{2}\pi)-f_2(\tfrac{1}{2}\pi)]\,, \tag{46}$$

where $f_n(\theta)$ denotes the nth term in the Born expansion for the scattering amplitude. Thus, the scattering amplitude itself becomes

$$f(\theta)=f_1(\tfrac{1}{2}\pi)f_1(\theta)/[\,f_1(\tfrac{1}{2}\pi)-f_2(\tfrac{1}{2}\pi)]\,, \tag{47}$$

which closely resembles the value for $f(\theta)$ found using the Schwinger variational principle[8] with plane-wave trial functions, namely,

$$f_{\mathrm{Sch}}(\theta)=f_1(\theta)^2/[f_1(\theta)-f_2(\theta)]\,. \tag{48}$$

Thus, even at lowest order, the results via collocation should be reasonable.

The linear equations that must be solved for x_i and y_i using collocation points v_j^2 are

$$R(v_j^2)=0=\sum_{i=0}^{N_v} x_i\psi_i(v_j)+\sum_{i=1}^{N_u} y_i\phi_i(v_j)-\psi_0(v_j) - c\left(x_0T_2(v_j^2)+\sum_{i=1}^{N_v} x_i\tilde{C}_i(v_j)+\sum_{i=1}^{N_u} y_i\tilde{S}_i(v_j)\right), \quad j=1,\ 2,\ \ldots,\ N \tag{49}$$

where $T_2(v)$, $\tilde{C}_i(v)$, and $\tilde{S}_i(v)$ are defined by

$$T_2(v)=\sum_{l=1}^{N_a}\sum_{l'=1}^{N_a} a_l a_{l'}\int d^3Q''\frac{e^{-t_l v_2^2}e^{-t_{l'}v_1^2}}{A^2-Q''^2+i\epsilon}, \tag{50}$$

$$\tilde{C}_i(v)=\sum_{l=1}^{N_a} a_l\int d^3Q''\frac{e^{-t_l v_2^2}e^{-\gamma v_1^2}\cos(\omega_i v_1^2)}{A^2-Q''^2+i\epsilon}, \tag{51}$$

$$\tilde{S}_i(v)=\sum_{l=1}^{N_a} a_l\int d^3Q''\frac{e^{-t_l v_2^2}e^{-\alpha u_1^2}\sin(\omega_i u_1^2)}{A^2-Q''^2+i\epsilon}. \tag{52}$$

The variables v_2^2, v_1^2, and u_1^2 are, as before, defined by Eqs. (28)–(30), respectively. The integrals in these functions have been evaluated analytically and the final expressions for $T_2(v)$, $\tilde{C}_i(v)$, and $\tilde{S}_i(v)$ are given in Appendix B.

To obtain the equations in the matrix form, it is convenient to define the functions

$$F_{j0}=\psi_0(v_j)-cT_2(v_j), \tag{53}$$

$$G_{ji}=e^{-\gamma v_j^2}\cos(\omega_i v_j^2)-c\tilde{C}_i(v_j), \tag{54}$$

$$H_{ji}=-\left[e^{\alpha v_j^2-4\alpha Q^2}\sin(\omega_i v_j^2)+cS_i(v_j)\right], \tag{55}$$

so that Eq. (49) becomes

$$x_0F_{j0}+\sum_{i=1}^{N_v} x_iG_{ij}+\sum_{i=1}^{N_u} y_iH_{ij}=\psi_0(v_j), \quad j=1,\ 2,\ \ldots,\ N. \tag{56}$$

Defining the matrices

$$\underline{D}=\begin{pmatrix} F_{10} & G_{11} & G_{12} & \cdots & G_{1N_v} & H_{11} & H_{12} & \cdots & H_{1N_u} \\ F_{20} & G_{21} & G_{22} & \cdots & & & & & \\ \vdots & & & & & & & & \\ F_{N0} & G_{N1} & G_{N2} & \cdots & G_{NN_v} & H_{N1} & H_{N2} & \cdots & H_{NN_u} \end{pmatrix}, \tag{57}$$

$$b=\begin{pmatrix} x_0 \\ x_1 \\ \vdots \\ x_{N_v} \\ y_1 \\ \vdots \\ y_{N_u} \end{pmatrix}, \tag{58}$$

and

$$s=\begin{pmatrix} \psi_0(v_1) \\ \psi_0(v_2) \\ \vdots \\ \psi_0(v_N) \end{pmatrix} \tag{59}$$

implies Eqs. (56) become

$$\underline{D}\,b=s \tag{60}$$

to be solved for the solution vector b.

For both matrix equations, (44) for the Hermite case and (60) for the sine-cosine expansion set, the conjugate gradient method[26] was used to obtain a solution vector and the largest matrix set considered was a 25×25 complex $\underline{D}$ matrix.

V. NUMERICAL RESULTS

The numerical calculations were performed using a five-term fit to the potential matrix representing a Yukawa potential in Eq. (16). Exact numerical results with the parameters $V_0=-53$ MeV and $A_0=1.35$ fm for neutron-proton scattering are available in the literature.[17–20] However, these parameters can be scaled to atomic units and the results are therefore presented in reduced units, namely, the scattering amplitude $f(\theta)$ in units of A_0, the differential cross section $d\sigma/d\Omega$ in units of A_0^2, and the total cross section σ_T in units of πA_0^2. The approximate nonperturbative T matrices obtained by solving Eqs. (44) or (60) were used to generate $f(\theta)$, $d\sigma(\theta)/d\Omega$, and σ_T as a function of the number of terms retained in the basis set. To obtain smooth results as a function of the number of terms retained, the solution vectors, at a given order N, were averaged as follows: The jth coefficient, e.g., $x_j^{(N)}$, in an expansion of order $N(j\le N)$ is linearly averaged with all values of $x_j^{(M)}$ obtained previously in expansions of order $M<N$. Thus, x_j^{av} is defined as

$$x_j^{\mathrm{av}}=(x_j^{(1)}+x_j^{(2)}+\cdots+x_j^{(N)})/N. \tag{61}$$

Of course, for $j>M$ the expansion coefficient is identically zero. The simplest example is $N=2$ for which

$$x_1^{\mathrm{av}}=\tfrac{1}{2}(x_1^{(1)}+x_2^{(2)}), \tag{62}$$

$$x_2^{\mathrm{av}}=\tfrac{1}{2}(x_2^{(1)}+x_2^{(2)}), \tag{63}$$

where $x_2^{(1)}=0$. The T matrix converges to the same result with averaged and unaveraged expansion coefficients, but the trends are more readily discovered using the averaging procedure.

Figures 2 and 3 illustrate typical results for the differential cross section using the SC-1 expansion in sines and cosines and illustrate that the basic properties of the differential cross section are re-

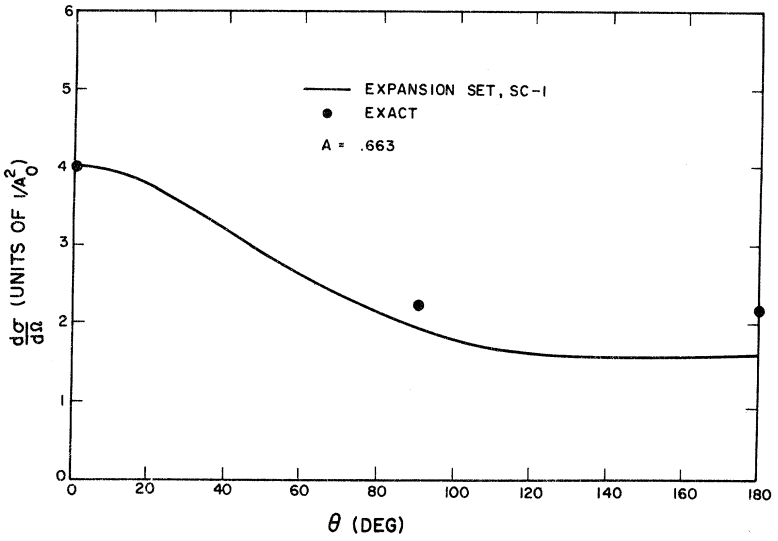

FIG. 2. Differential cross section using SC-1 basis-set expansion for T; $A = 0.663$.

produced. These results were obtained using α and γ equal to zero. Similar results were found for $\alpha = \gamma = 0.01$, but for larger values of α and γ, such as 0.1 or larger, the results were less accurate. This sensitivity is most likely related to the fact that for large values of α and γ, the linear independence of the expansion functions, in particular over the on-shell range, is masked by the strongly decaying Gaussians. The phase information obtained is illustrated in Fig. 4, where the real and imaginary parts of the scattering amplitude at $\theta = 0$ are shown along with the exact value.[28] Of course, there is no phase information of $f(\theta)$ in the Born approximation. This phase information leads to an optical theorem value of σ_T^{op}, which is compared with σ_T^{int}, obtained by integration of $d\sigma/d\Omega$, in Fig. 5. The results both converge to within 10% or less of the exact results indicating approximate unitarity is preserved. The wide variations in the low-N results are most likely due to the solution scheme since only N collocation points are required to obtain the expansion coefficients, yet with only a few collocation points one can expect wide variations in the residual function from zero. The values of σ_T^{int} and σ_T^{op} do not converge to each other or to the exact answer because the expansion functions themselves are not complete in the space of T. That the results are physically reasonable supports the choice of u^2 and v^2 and the neglect of the $\vec{u} \cdot \vec{v}$ variable, which is zero on shell.

Typical results for the differential cross sections obtained using the Hermite expansion H-1 for T are shown in Figs. 6 and 7. Again, the basic physical features of the cross section are adequately repro-

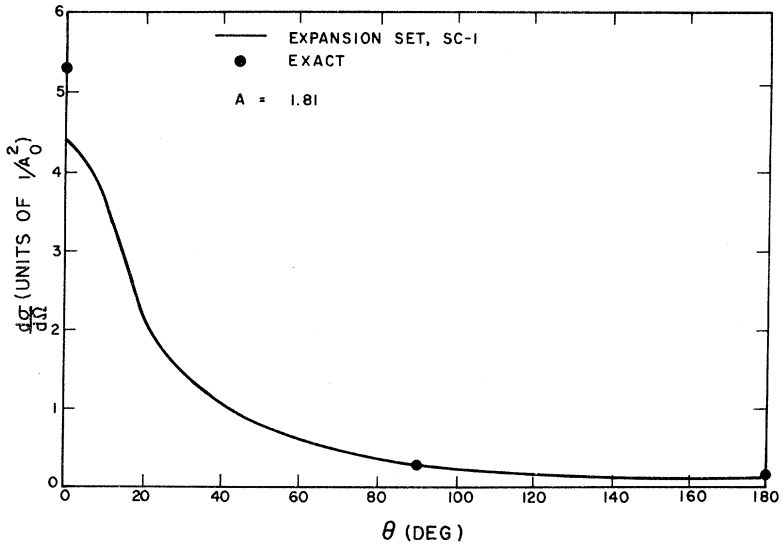

FIG. 3. Differential cross section using SC-1 basis-set expansion for T; $A = 1.81$.

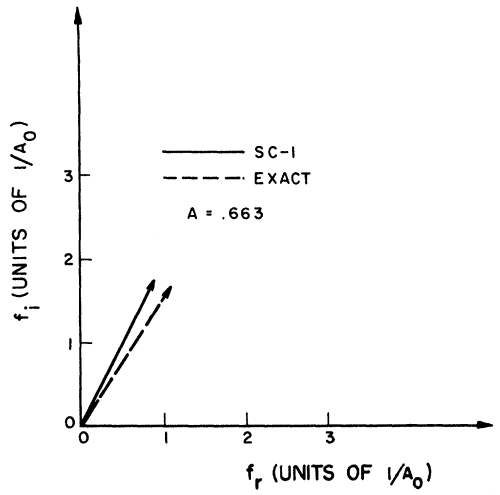

FIG. 4. Real and imaginary parts of the scattering amplitude $f(\theta)$ obtained using the SC-1 expansion set in the forward direction when $A = 0.663$. The first Born approximation gives $f_{im}(\theta) = 0$.

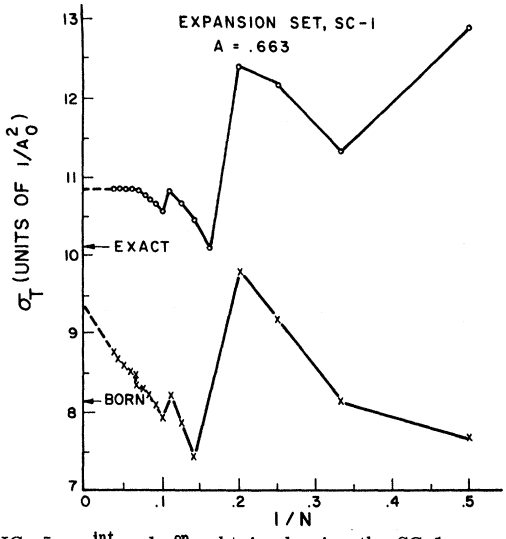

FIG. 5. σ_T^{int} and σ_T^{op}, obtained using the SC-1 expansion set, vs $1/N$, where N is the number of terms retained in the basis set.

duced in both the forward and backward hemispheres and, as well, phase information on $f(\theta)$ is obtained,[28] as shown in Fig. 8. The results were obtained using $\alpha = \gamma = 0.01$. As discussed above, values of α and γ greater than 0.1 led to poorer results because the linear independence of the expansion functions, in particular over the on-shell range, becomes masked by the strong damping of the Gaussian. On the other hand, α and γ cannot be zero because finite values are required to obtain convergent integrals using the Galerkin method. A typical convergence plot for the expansion set H-1 is shown in Fig. 9, and the smoothness, in contrast to Fig. 5 for the SC-1 expansion, is due to the use of the Galerkin method, which sets a weighted integral of the residual equal to zero. Therefore, comparable accuracy can be obtained using fewer terms in the expansion H-1 as compared to SC-1. As before, however, the values of σ_T^{int} and σ_T^{op} do not converge to each other but both are close to the exact result. This again results from the incompleteness of the expansion set in the space of T, but the adequacy of the results indicates the expansion set spans the most important part of T space. This is more clearly seen by comparison with expansion set H-2 [Eq. (21)] which is an expansion in functions that depend only on v^2. The results for $d\sigma/d\Omega$ are shown in Fig. 7 together with the results

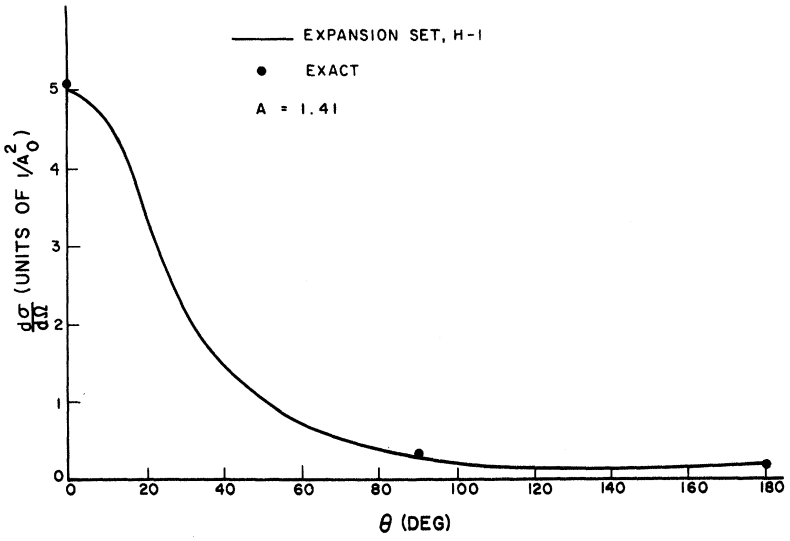

FIG. 6. Differential cross section using the Hermite polynomial basis set H-1; $A = 1.41$.

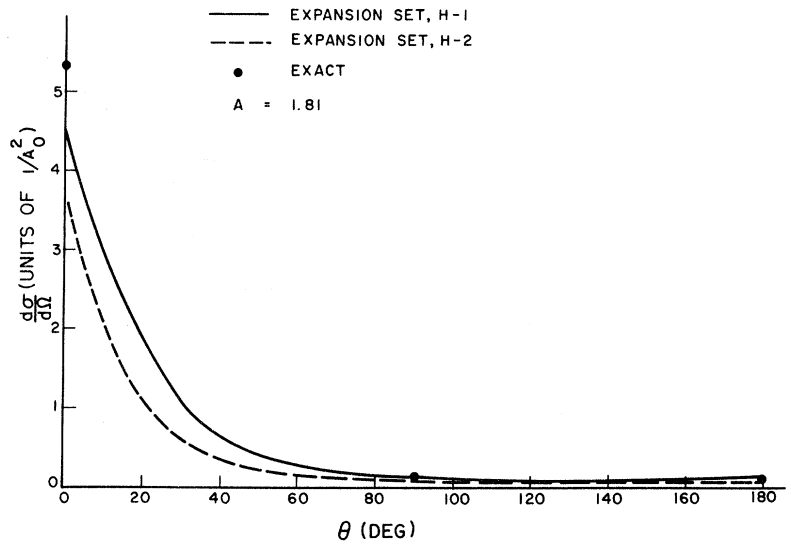

FIG. 7. Differential cross sections obtained using the H-1 and H-2 basis-set expansions of T; $A=1.81$. The H-2 basis set uses only the v^2 variable.

using expansion set H-1 (with v^2 and u^2 variables). It is clear both in Fig. 7 and in the convergence plot Fig. 10 that the use of u^2 variables is quite important and its absence leads to converged results that are not as good as those obtained using v^2 and u^2. Also, the variables u^2 and v^2 seem adequate to reproduce the essential physics even in energy ranges far from the Born limit, such as $A=0.663$ and 1.41, and they are clearly superior to the use of v^2 alone. The use of the $\vec{u}\cdot\vec{v}$ variable would probably improve results even more, but this effort does not seem warranted within the context of what we are looking for.

It is also interesting that the number of terms in the basis sets required to achieve similar accuracies in σ_T remained essentially independent of energy over the energy range studied. This is in contrast to solution methods, such as partial waves,[8] which require an ever-increasing number of terms as the energy increases. The expansion sets SC-1 and H-1 have also been able to reproduce reasonably well the variation of σ_T with energy. This is shown in Table I, where σ_T is given as a function of A $(=kA_0)$ and V_0/E.

VI. CONCLUSIONS

The results presented indicate that reasonable approximate results can be achieved on three-dimensional scattering problems when a suitable choice of "characteristic variables" is made and a nonperturbative basis-set expansion that fits the shape of the T matrix is chosen. The results are sensitive to the choice of variables, as indicated by the results using only v^2 variables rather than both v^2 and u^2. The results have provided some insight into the method for choosing such variables;

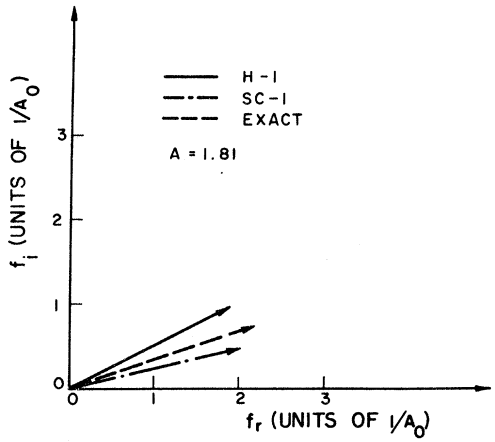

FIG. 8. Real and imaginary part of $f(\theta)$, the $\theta=0$, obtained using the H-1 and SC-1 expansion sets; $A=1.81$. The Born approximation gives $f_{\mathrm{im}}(\theta)=0$.

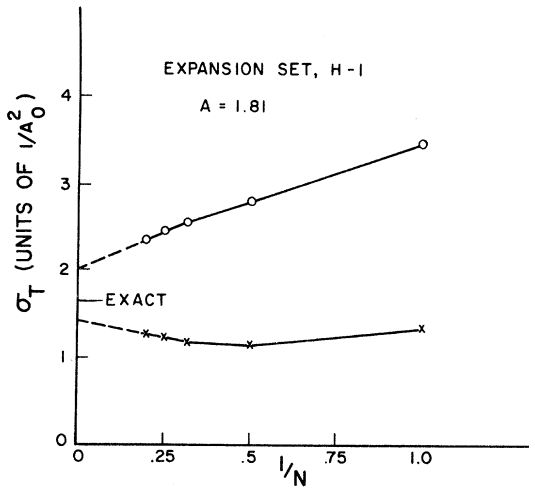

FIG. 9. σ_T^{int} and σ_T^{op} from the H-1 expansion set.

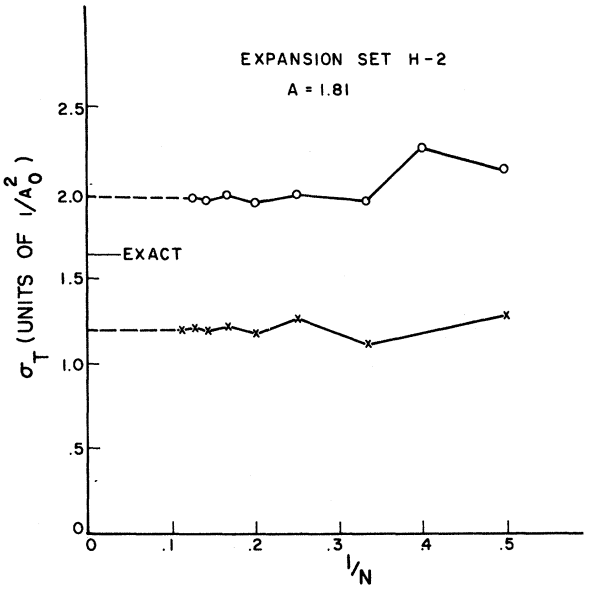

FIG. 10. σ_T^{int} and σ_T^{op} from the H-2 expansion set vs $1/N$, where N is the number of terms in the expansion.

in particular, the characteristic variables of the V matrix seem to remain important variables for T. Also, variables dominant near the on-shell range are especially important. This is illustrated by our ability to achieve reasonable results using only v^2 and u^2 variables (neglecting $w = \vec{u} \cdot \vec{v}$) and by the effort to synthesize T from expansions that did not involve products of functions of v^2 and functions of u^2. Certainly, the results can be improved by including the w variable and including product functions, but our results indicate the improvement will not exceed 10% or so. Further, we clearly have not expanded in basis sets that are complete in the space of T, but again the adequacy of the results indicates one can, by choosing appropriate variables, apparently span the most important part of that space. We have also noted that the number of terms required in the basis set after which one can safely extrapolate to the converged result seems relatively insensitive to the energy. This reflects the nonperturbative nature of the approach. All this information, together with the knowledge gained in the previous paper,[6] will be important when, as is now being done, the approach is extended to three-dimensional problems with inelasticity and many open channels.

As a final point, we should like to place these results in a different perspective than the one used heretofore. In the current context, this paper is aimed at examining whether adequate approximations to the T matrix could be obtained in a three-dimensional problem by fitting the shape of T. The expansion coefficients for T were found by some variant of the weighted-residuals method and the physical information, namely, cross sections, were directly derived. However, it is also possible to consider the MS approach as a scheme for generating approximate nonperturbative T matrices which can be used as trial functions in a stationary principle for T to derive even more adequate values for the transition matrix. This is in contrast to the more standard variational approaches[29] which generally involve the evaluation of trial wave functions for use in stationary expressions for T. The Schwinger principle is an example of this approach.[7] In fact, two such stationary expressions for T in the form we require are available.[30] We are currently extending the variational approach to couple it with the MS method for both elastic and inelastic problems so that the entire method can be placed on a firmer mathematical foundation. To this date, we have investigated elastic scattering using the variational approach and the results are very promising.[31,32]

Note added in manuscript. The authors recently received a preprint entitled "Scattering Amplitude Calculated with Continuous Space-filling Curves," by C. M. Rosenthal and D. J. Kouri, which is closely related to the material in this paper.

APPENDIX A

The functions $W_i^{\pm}$ ($i = 1$, 2, 3, and 4) are required in order to solve for the expansion coefficients in the Hermite polynomial basis-set expansion of T. The elements S_{nj} of Eq. (39) are defined in terms of the functions $W_1^{\pm}(n, \frac{1}{2}j)$ and $W_2^{\pm}(n, \frac{1}{2}(j-1))$ which, in turn, can all be expressed in terms of a function $X_{a,b}(\beta)$, defined as

$$X_{a,b}(\beta) = \int_0^\infty 4\pi y^2 \, dy \, e^{-\beta y^2} H_{a-1}(y^2) H_{b-1}(y^2), \quad \text{(A1)}$$

where a and b are integers. Using the recursion relation for Hermite polynomials,[22] one can show that the X functions satisfy the recursion formula

$$X_{a,b}(\beta) = X_{a-1,b+1}(\beta) - 2(a-2)X_{a-2,b}(\beta) + 2(b-1)X_{a-1,b-1}(\beta). \quad \text{(A2)}$$

Further, $X_{a,b}$ is symmetric, i.e.,

$$X_{a,b}(\beta) = X_{b,a}(\beta). \quad \text{(A3)}$$

Using (A1) and (A2), it is possible to evaluate all the X functions if one knows $X_{1,b}(\beta)$ for all b.

TABLE I. Total cross section—variation with energy.

A	V_0/E	σ_T^{int} expansion SC-1	σ_T^{int} expansion H-1	σ_T first Born approx.	σ_T (exact)
0.663	5.38	9.40	9.25	8.12	10.09
1.406	1.19	2.79	2.55	2.51	2.639
1.816	0.716	1.80	1.45	1.58	1.628
3.0	0.262	0.562	0.635	0.601	0.59

The functions $X_{1,b}(\beta)$ can be evaluated by first making the variable change $x=\beta y^2$, so that Eq. (A1) becomes, for $X_{1,b}(\beta)$,

$$X_{1,b}(\beta)=(2\pi/\beta^{3/2})\int_0^\infty x^{1/2}dx\,e^{-x}H_{b-1}(x/\beta). \quad \text{(A4)}$$

Carrying out the integral gives

$$X_{1,b}(\beta)=\pi 2^b\sum_{m=1}^{[1/2(b-1)]+1}\frac{(b-1)!\,\Gamma(\frac{5}{2}+b-2m)\beta^{2m-b-5/2}(-1)^{m-1}}{(m-1)!(b+1-2m)!\,2^{2m-2}}, \quad \text{(A5)}$$

where $[z]$ stands for "greatest integer less than or equal to z," and Γ is the gamma function.[21] In terms of the X function, the $W_i^\pm$ functions for $i=1$ and 2 become

$$W_1^+(n,\ \tfrac{1}{2}j)=\sum_{l=1}^{N_a}a_l X_{1,(n+1)/2}(t_l)X_{1,j/2}(2\alpha), \quad \text{(A6)}$$

$$W_1^-(n,\ \tfrac{1}{2}j^-)=X_{1,1}(1)X_{n/2,j/2}(2\alpha), \quad \text{(A7)}$$

$$W_2^+(n,\ \tfrac{1}{2}(j-1))=X_{1,1}(\alpha)\sum_{l=1}^{N_a}\sum_{l'=1}^{N_a}a_l a_{l'}X_{(n+1)/2,(j-1)/2}(t_l+t_{l'}), \quad \text{(A8)}$$

$$W_2^-(n,\ \tfrac{1}{2}(j-1))=\sum_{l=1}^{N_a}a_l X_{n/2,1}(\alpha)X_{1,(j-1)/2}(1+t_l). \quad \text{(A9)}$$

The matrix elements C_{nj}, defined in terms of functions $W_3(n,\ \frac{1}{2}j;\ l)$ and $W_4^\pm(n,\ \frac{1}{2}(j-1);\ l)$, can also be evaluated analytically but the derivation is extremely tedious and we spare the reader the details. In short, the functions $W_3^\pm$ and $W_4^\pm$ can be expressed in terms of a function $F_{ik}(\xi,\ l;\ A)$, where $A=kA_0$ as before, and ξ will be defined. The integrations were performed by interchanging orders of integration, performing the $d^3u\,d^3v$ integrals first, and then carrying out the integral over d^3Q''. The final expression for the function $F_{ik}(\xi,\ l;\ A)$ is

$$\begin{aligned}F_{ik}(\xi,\ l;\ A)=&\frac{64\pi^5 f^{1/2}}{(2fd+gh)(4fc-h^2)}\sum_{\bar m=0}^{k}\frac{\tilde S_{\bar m}(1/4f,\ k)\bar m!}{f^{\bar m}}\left(\frac{(2f+h)^2 4f}{4fc-h^2}\right)^{\bar m}\sum_{r=0}^{\bar m}\frac{(-1)^r[2(\bar m-r)]!}{(\bar m-r)!}\left(\frac{(4f+g)(4fc-h^2)}{(2fd+gh)(2f+h)}\right)^r\\
&\times\sum_{\bar m'=0}^{i}\tilde S_{\bar m'}\left(\frac{4f}{4fc-h^2},\ i\right)(2\bar m'+1)!\sum_{s_1=1}^{\bar m'+\bar m+1-r}\left(\frac{(4f+g)(4fc-h^2)+(2f+h)(2fd+gh)}{(2f+h)[4f(4fc-h^2)]^{1/2}}\right)^{2s_1-1}\\
&\times\sum_{j=1}^{s_1}\frac{A^{(s_1-j)}(-1)^{s_1+j}(s_1+j-2)!}{(2\xi^{1/2})^{s_1+j-1}(s_1-j)!(j-1)!}\quad((-1)^{1/2}w(\xi^{1/2}A))^{s_1+1-j}\\
&\times\sum_{p=0}^{2s_1-1}2^{2(\bar m'+r+s_1-\bar m)}\frac{\{(2fd+gh)(2f+h)/[(4f+g)(4fc-h^2)+(2f+h)(2fd+gh)]\}^p}{2^p p!(2s_1-1-p)!(2\bar m'+1-p)!(p+\bar m-s_1-r-\bar m')!}H(\bar m+p-\bar m'-r-s_1)\\
&\times H(2\bar m'+1-p)H(2\bar m-2r+2s_1+p+1), \quad \text{(A10)}\end{aligned}$$

where

$$\tilde S_m(a,\ n)=\frac{n!}{2(2m+1)!}\sum_{t=0}^{[n/2]}\frac{(-1)^t(2n-4t+1)!(\frac{1}{2}a)^{n-2t}H(n-m-2t)}{t!(n-2t)!(n-m-2t)!}. \quad \text{(A11)}$$

H stands for the Heaviside function and $w(z)$ is a standard function[21] related to the error function and defined, for complex z, by

$$w(z)=\frac{i}{\pi}\int_{-\infty}^{\infty}\frac{e^{-t^2}}{z-t}dt=e^{-z^2}\operatorname{erfc}(-iz),\quad \operatorname{Im}(z)>0. \quad \text{(A12)}$$

In terms of $F_{ij}(\xi,\ l;\ Q)$, the functions $W_3^\pm$ and $W_4^\pm$ become

$$W_3^+(n,\ \tfrac{1}{2}j;\ l)=\sum_{l''=1}^{N_a}a_{l''}F_{(n+1)/2,j/2}(\xi_1,\ l;\ A), \quad \text{(A13)}$$

$$W_3^-(n,\ \tfrac{1}{2}j;\ l)=F_{n/2,j/2}(\xi_1,\ l;\ A), \quad \text{(A14)}$$

$$W_4^+(n,\ \tfrac{1}{2}(j-1);\ l)=\sum_{l_2^{\prime\prime}=1}^{N_a}\sum_{l_2^{\prime\prime\prime}=1}^{N_a}a_{l_2^{\prime\prime}}a_{l_2^{\prime\prime\prime}}F_{(n+1)/2,(j-1)/2}(\xi_4,\ l;\ A), \quad \text{(A15)}$$

$$W_4^-(n,\ \tfrac{1}{2}(j-1);\ l)=\sum_{l'''=1}^{N_a}a_{l'''}F_{n/2,(j-1)/2}(\xi_4,\ l;\ A), \quad \text{(A16)}$$

where the arguments ξ_1 and ξ_4 are defined as

$$\xi_m=\sigma_m-\frac{1}{4f}\left(g^2+\frac{(2fd+gh)^2}{4fc-h^2}\right),\quad m=1,\ 4. \quad \text{(A17)}$$

The factors c, d, f, g, and h are given in Table II for each function. The constants σ_1 to σ_5 in the table are

$$\sigma_1=t_l+\alpha, \quad \text{(A18a)}$$

$$\sigma_2=\tfrac{1}{4}(5\alpha+t_l), \quad \text{(A18b)}$$

TABLE II. Arguments in $W_i^{\pm}$.

	c	d	f	g	h
W_3^+	$\frac{1}{4}\sigma_1+\gamma$	$-\sigma_1$	σ_2	$-\sigma_3$	$-\frac{1}{2}\sigma_3$
W_3^-	σ_2	$-\sigma_3$	$\frac{1}{4}\sigma_1+\gamma$	$-\sigma_1$	$-\frac{1}{2}\sigma_3$
W_4^+	$\frac{1}{4}\sigma_4+\gamma$	σ_5	$\frac{1}{4}\sigma_4+\alpha$	$-\sigma_4$	$\frac{1}{2}\sigma_5$
W_4^-	$\frac{1}{4}\sigma_4+\alpha$	$-\sigma_4$	$\frac{1}{4}\sigma_4+\gamma$	σ_5	$\frac{1}{2}\sigma_5$

$$\sigma_3=\alpha-t_l\,, \tag{A18c}$$

$$\sigma_4=t_l+t_{l''}\,, \tag{A18d}$$

$$\sigma_5=t_l-t_{l''}\,. \tag{A18e}$$

Using (A10) together with (A17), (A18), and Table II, the functions $W_3^{\pm}$ and $W_4^{\pm}$ are evaluated.

APPENDIX B

When sine-cosine expansion set and collocation are used, the functions $T_2(v_j)$, $\tilde{C}_m(v_j)$, and $\tilde{S}_m(v_j)$, with v_j on shell, must be evaluated. Each function can be expressed in terms of a function $I^{\pm}(r,\ s)$ of two complex variables (r and s), defined by the integral

$$I^{\pm}(r,\ s)=\int d^3q''\,\frac{e^{-[(\vec{q}'-\vec{q}'')/4r]}e^{-[(\pm\vec{q}-\vec{q}'')^2/4s]}}{A^2-q''^2+i\epsilon}\,, \tag{B1}$$

where $\vec{q}=\vec{k}A_0$ and $A=|\vec{q}|$. Such integrals have been considered previously[15] for real arguments r and s. The evaluation for complex r and s can be carried through in a similar way to yield, for $\mathrm{Re}(1/r+1/s)>0$,

$$I^{\pm}(r,\ s)=\frac{2i\pi^2 rs}{|s\vec{q}'\pm r\vec{q}|}\,e^{-(\pm\vec{q}-\vec{q}')^2/4(r+s)}$$

$$\times\left\{w\left[\frac{A}{2}\left(\frac{r+s}{rs}\right)^{1/2}+\frac{|s\vec{q}'\pm r\vec{q}|}{2[rs(r+s)]^{1/2}}\right]\right.$$

$$\left.-w\left[\frac{A}{2}\left(\frac{r+s}{rs}\right)^{1/2}-\frac{|s\vec{q}'\pm r\vec{q}|}{2[rs(r+s)]^{1/2}}\right]\right\}\,, \tag{B2}$$

where $w(z)$ is defined by (A12) and where, for r and s complex, we define $|s\vec{q}'\pm rq|=(s^2q'^2+r^2q^2\pm 2rs\vec{q}'\cdot\vec{q})^{1/2}$. In terms of $I^{\pm}(r,\ s)$, the three functions of interest are

$$T_2(v)=\sum_{l=1}^{N_q}\sum_{l'=1}^{N_q}a_l a_{l'}I^{+}\left(\frac{1}{4t_{l'}}\,,\frac{1}{4t_l}\right)\,, \tag{B3}$$

$$\tilde{C}_m(v)=\sum_{l=1}^{N_q}\frac{a_l}{2}\left[I^{+}\left(\frac{1}{4t_l}\,\frac{1}{4(\gamma-i\omega_m)}\right)\right.$$

$$\left.+I^{+}\left(\frac{1}{4t_l}\,,\frac{1}{4(\gamma+i\omega_m)}\right)\right]\,, \tag{B4}$$

$$\tilde{S}_m(v)=\sum_{l=1}^{N_q}\frac{a_l}{2i}\left[I^{-}\left(\frac{1}{4t_l}\,,\frac{1}{4(\alpha-i\omega_m)}\right)\right.$$

$$\left.-I^{-}\left(\frac{1}{4t_l}\,,\frac{1}{4(\alpha+i\omega_m)}\right)\right]\,, \tag{B5}$$

where, on shell, $|\vec{q}|=|\vec{q}'|$, $v^2=2A^2(1-\cos\theta)$, and $u^2=2A^2(1+\cos\theta)$ for θ the scattering angle in the center-of-mass system.

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