Techniques for heavy-ion coupled-channels calculations. II. Iterative solution of the coupled radial equations

M. Rhoades-Brown, M. H. Macfarlane, and Steven C. Pieper
Argonne National Laboratory, Argonne, Illinois 60439
(Received 26 November 1979)

This paper, the second in a series on techniques for heavy-ion coupled-channels calculations, compares various iterative methods for the solution of the coupled radial equations in the interior region of configuration space. We consider the Born-Neumann series, sequential iteration, the method of moments, and Austern's modification of the Sasakawa method. The use of Padé approximants is shown to eliminate convergence problems with Born and sequential iteration. We conclude that sequential iteration with Padé acceleration is the most rapidly convergent and most efficient way of carrying out coupled-channels calculations for heavy-ion inelastic scattering; 0.5% accuracy in cross sections can be achieved with three or four iterations in each partial wave.

[NUCLEAR REACTIONS HI coupled-channels inelastic scattering. Iterative solution of radial equations.]

I. INTRODUCTION

Coupled-channels calculations for the inelastic scattering of heavy ions have been severely restricted by their computational complexity. Major souces of difficulty include (1) the long range of the Coulomb coupling potential, (2) the large number of channels that must be considered, and (3) the large number of partial waves that contribute significantly. The efficient treatment of Coulomb coupling was discussed in the first paper[1] of this series. It was shown that the Alder-Pauli[2] decomposition of the coupled-channels Coulomb wave functions allows efficient computation of incoming and outgoing solutions of the coupled radial equations in the region $r > R_N$, where R_N is a radius at which nuclear potentials are no longer important ($R_N \sim 20$–30 fm). These coupled-channels Coulomb functions replace the standard Coulomb functions in the process of extracting S-matrix elements. Thus it is possible to stop the outward integration of the interior radial equations at R_N instead of the several-hundred-fm radius that would be necessary if the Coulomb coupling were not explicitly treated.

In the present paper we discuss methods for solving the coupled equations in the region $r < R_N$, i.e., where both nuclear and Coulomb forces are important. For Coulomb-dominated reactions it is possible to avoid explicit treatment of an interior region by use of the Alder-Pauli[2] approach for all significant r values. However, in the presence of strong nuclear interactions most of the approximations used to simplify the equations of the Alder-Pauli method break down; we therefore prefer to solve the original radial equations directly.

The traditional method is to solve the N coupled equations, from $r = 0$ to $r = R_N$, N times with linearly independent starting values. A linear combination of the resulting N sets of regular solutions may then be found that has the desired boundary conditions as $r \to \infty$ (incoming and outgoing waves in the elastic channel, outgoing waves in all other channels). In this process the complete $N \times N$ S matrix can be extracted even though only one column is needed to compute the desired cross sections.

This procedure is reasonable for light-ion calculations where the number of coupled equations is usually moderate ($N \lesssim 20$). In heavy-ion studies much larger systems of coupled equations are encountered and it is no longer feasible to solve the N coupled equations N times (thus computing N^2 radial wave functions) in order to extract the single desired column of the S matrix.

A number of iterative procedures have been introduced in attempts to reduce the amount of computational labor. All involve recursive solution for a single set of radial wave functions that are constrained to have the desired boundary conditions. The aim is to construct a converged solution in a reasonable number of iterations. In this paper we compare several of these schemes and discuss their efficiency for heavy-ion reactions.

The most obvious scheme is to generate the Born-Neumann series for the wave functions and S matrices. We refer to this as "block iteration" since the wave functions in all channels are treated together in a block. Raynal[3] has suggested a variant of this method in which the radial equations are treated one at a time in a definite sequence rather than as a block; improvements in the solutions of the equations that occur earlier in

the sequence are then incorporated in the equations to be solved later in the sequence. This is referred to as "sequential iteration." We find that it has substantially better convergence properties than block iteration.

Both of these methods build up the wave functions and S matrices as power series in the coupling potential and both can diverge for physically reasonable potentials. As was suggested by Raynal[3] one can use Padé approximants to accelerate the convergence of the S matrices for both schemes. The Padé approximants to these power series are rational functions that have a larger radius of convergence and may converge when the original series diverges. Furthermore, if block iteration is used, the Padé approximants yield the S-matrix elements as rational functions of the overall coupling strength. This permits the coupling strength to be fitted to data in about the same time as it takes to do a calculation for a single coupling strength.

Other iterative techniques have been proposed that also express the S-matrix elements as rational functions of the coupling strength. One is the method of moments, recently studied for proton inelastic scattering by Griffin and Koshel.[4] It has been proved to converge for a wide class of potentials—certainly wide enough to include any potential likely to be encountered in heavy-ion studies. We find that for heavy-ion inelastic scattering, the moment method converges markedly more slowly than sequential iteration with Padé acceleration.

We also consider a variant, proposed by Austern,[5] of the Sasakawa[6,7] method. The modified procedure has no guaranteed convergence properties and fails to converge in some of our tests. While it is more reliable than straightforward block iteration, it is significantly slower than either block or sequential iteration with Padé acceleration. The multichannel implementation[3] of the original Sasakawa method, which does have proved convergence properties,[7] involves much more computational labor than the brute force solution of the original coupled equations and is therefore not practical.

In Sec. II we describe in more detail the methods of iteration outlined above. Numerical comparisons of the techniques are presented in Sec. III; iterative solution of the Alder-Pauli equations for all values of r is discussed in Sec. IV; and our conclusions are summarized in Sec. V.

II. ITERATIVE TECHNIQUES FOR THE COUPLED RADIAL EQUATIONS

The radial equations to be solved, in the notation established in paper I[1] of this series, are

$$D_\alpha(r)R_\alpha(r)=\sum_{\beta=1}^{N} U_{\alpha\beta}(r)R_\beta(r) \quad (\alpha=1,2,\ldots,N), \tag{2.1}$$

where

$$D_\alpha(r)=\frac{d^2}{dr^2}-\frac{l_\alpha(l_\alpha+1)}{r^2}-U_\alpha^{\rm opt}(r)+k_\alpha{}^2. \tag{2.2}$$

These equations refer to a single value (J,π) of the total angular momentum and parity of the system; we suppress the labels (J,π). The solutions R_α of Eq. (2.1) are to be regular at the origin and have the asymptotic form

$$R_\alpha(r)\underset{r\to\infty}{=}\frac{i}{2}\left[I_{\alpha_0}(r)\delta_{\alpha\alpha_0}-\left(\frac{k_{\alpha_0}}{k_\alpha}\right)^{1/2}S_{\alpha\alpha_0}O_\alpha(r)\right], \tag{2.3}$$

where I_α and O_α are incoming and outgoing Coulomb functions and $S_{\alpha\alpha_0}$ are the desired S-matrix elements. The channel with an incoming wave is indicated by α_0.

Use of the asymptotic form (2.3) requires integration of the radial equations out to distances beyond which Coulomb coupling terms are negligible—several hundred fm for many heavy-ion reactions. As discussed in paper I, use of the modified asymptotic form

$$R_\alpha(r)\underset{r\to\infty}{=}\frac{i}{2}\left[\mathcal{I}_{\alpha_0,\alpha}(r)-\sum_\beta\left(\frac{k_{\alpha_0}}{k_\beta}\right)^{1/2}S_{\beta\alpha_0}\mathcal{O}_{\beta,\alpha}(r)\right], \tag{2.4}$$

where $\mathcal{I}_{\beta,\alpha}$ and $\mathcal{O}_{\beta,\alpha}$ are incoming and outgoing *coupled-channels* Coulomb functions, permits matching to the interior solutions at the much-smaller nuclear matching radius R_N.

We shall make frequent use of the regular solutions f_α of the homogeneous parts of Eqs. (2.1). These regular or optical-model solutions satisfy

$$D_\alpha(r)f_\alpha(r)=0, \tag{2.5}$$

with

$$f_\alpha(r)\underset{r\to\infty}{=}\tfrac{1}{2}i\left[I_\alpha(r)-S_\alpha O_\alpha(r)\right], \tag{2.6}$$

where S_α is the optical-model S-matrix element in channel α. The solutions $R_\alpha(r)$ of the coupled equations (2.1), the optical-model solutions $f_\alpha(r)$ and the S-matrix elements $S_{\alpha\alpha_0}$ and S_α, satisfy an integral identity,

$$S_{\alpha\alpha_0}=\delta_{\alpha\alpha_0}S_\alpha-\frac{2i}{(k_\alpha k_{\alpha_0})^{1/2}}\sum_\beta\int f_\alpha(r)U_{\alpha\beta}(r)R_\beta(r)dr, \tag{2.7}$$

which will be used in our discussion of some of the

iterative techniques.

In this section we discuss a number of iterative techniques for the solution of Eqs. (2.1). All of them involve replacement of the system (2.1) of coupled equations by sets of uncoupled inhomogeneous equations

$$D_\alpha R_\alpha(r) = \phi_\alpha(r) \quad (\alpha = 1, 2, \ldots, N), \tag{2.8}$$

with driving terms specified by the known functions ϕ_α. The numerical solution of these equations proceeds in the following fashion. Let Z_α be a particular solution obtained by numerical integration starting with $Z_\alpha = 0$ at $r = 0$ (or at some finite value of r at which Z_α is negligibly small) and an arbitrary choice for $(d/dr)Z_\alpha$. The most general regular solution in channel α is obtained by adding an arbitrary multiple of the regular solution f_α of the homogeneous equation

$$R_\alpha(r) = Z_\alpha(r) + c_\alpha f_\alpha(r). \tag{2.9}$$

Substitution of Eq. (2.9) in the matching equations [Eqs. (2.4) and their r derivatives] yields a set of $2N$ inhomogeneous linear equations for the coefficients c_α and the S-matrix elements $S_{\alpha\alpha_0}$.

A. Block and sequential iteration

We first consider the most straightforward of iterative methods for the solution of Eqs. (2.1). Suppose that $k-1$ iterative steps have been completed, yielding a set of radial solutions $R_\alpha^{(k-1)}(r)$. These radial functions are used to construct the kth approximation to the solutions by solving the set of N uncoupled inhomogeneous equations

$$D_\alpha R_\alpha^{(k)} = \sum_\beta U_{\alpha\beta} R_\beta^{(k-1)}, \tag{2.10}$$

using the numerical procedure outlined above. The corresponding S-matrix elements $S_{\alpha\alpha_0}^{(k)}$ are obtained by solution of the matching equations. The new radial wave functions $R_\alpha^{(k)}$ are then substituted in the right-hand side of Eqs. (2.10) and the procedure iterated until convergence to a certain preassigned accuracy is achieved. As a criterion for convergence, we demand that the maximum (over channels α) of the magnitudes $|S_{\alpha\alpha_0}^{(k)} - S_{\alpha\alpha_0}^{(k-1)}|$ be less than some pre-assigned absolute error. Various initial estimates $R_\alpha^{(0)}$ may be used to start the iterative procedure. We have found that the precise choice of starting estimate is rather unimportant and therefore use the optical-model solution in the incoming channel:

$$R_\alpha^{(0)} = \delta_{\alpha\alpha_0} f_{\alpha_0}. \tag{2.11}$$

This iterative procedure, wherein at each stage all channels are treated in the same way and at the same level of approximation, we refer to as "block iteration." Each iteration generates one more term of the Born series for the S matrix and the wave functions. Because of this it is particularly ill suited for reactions in which a high-spin state can be reached only by a sequence of excitations of low multipolarity. For example in considering the population of a $J^\pi = 20^+$ state by successive 2^+ excitations, the desired S-matrix element will be zero for the first nine iterations of the block method.

Raynal[3] has proposed that the iterative scheme outlined above be carried out sequentially. The basic idea of sequential iteration is to solve the N inhomogeneous equations (2.10) in some definite order; each improved solution $R_\alpha^{(k)}(r)$ is immediately inserted in the inhomogeneous term of subsequent equations.

Each step of sequential iteration incorporates many effects absent in block iteration. Suppose that the channels α are ordered in some fashion with the elastic channel α_0 first, channels most strongly coupled to α_0 next, and so on, with channels that are strongly coupled grouped close to each other. The equations to be solved, in order, are then

$$D_\alpha R_\alpha^{(k)} = \sum_{\beta<\alpha} U_{\alpha\beta} R_\beta^{(k)} + \sum_{\beta>\alpha} U_{\alpha\beta} R_\beta^{(k-1)}, \tag{2.12}$$

for $\alpha = 2, 3, \ldots, N$, and for the elastic channel $(\alpha_0 = 1)$

$$D_1 R_1^{(k)} = \sum_{\beta=2}^{N} U_{1\beta} R_\beta^{(k)}. \tag{2.13}$$

As the iteration progresses through the channels, the initial guesses $R_\alpha^{(k-1)}$ are gradually replaced in the inhomogeneous terms by improved solutions $R_\alpha^{(k)}$. It is clear that higher-order corrections are thereby introduced that are absent from the corresponding stage of block iteration. In the example mentioned previously, the S-matrix element for the 20^+ state is nonzero in the first iteration with the appropriate ordering of channels.

The matching equations [Eq. (2.4) and its r derivative, with Eq. (2.9)] are also modified. In generating the solution $R_\alpha^{(k)}$ in channel α, the expansion coefficients $c_\beta^{(k)}$ and S-matrix elements $S_{\beta\alpha_0}^{(k)}$ in all other channels $\beta \neq \alpha$ are to be regarded as fixed; this yields a pair of simultaneous linear equations for $c_\alpha^{(k)}$, $S_{\alpha\alpha_0}^{(k)}$. Thus the $2N$ linear equations of block iteration are replaced in sequential iteration by N successively solved sets of two linear equations.

B. Padé approximants

It is found that, for heavy-ion as for light-ion reactions, sequential iteration provides signifi-

cantly better convergence than block iteration; this will be shown in Sec. III. Nevertheless there are many interesting heavy-ion reactions for which sequential iteration diverges. As was suggested by Raynal,[3] the convergence problems of either block or sequential iteration can be overcome with the aid of Padé approximants. Suppose that an iterative procedure yields a sequence

$$S^{(0)}, S^{(1)}, S^{(2)}, \ldots, S^{(k)} \tag{2.14}$$

of approximations to a certain S-matrix element

$$S = S_{\alpha\alpha_0}. \tag{2.15}$$

We define a set of coefficients b_r by the relations

$$\begin{aligned} b_0 &= S^{(0)}, \\ b_1 &= S^{(1)} - S^{(0)}, \\ b_2 &= S^{(2)} - S^{(1)}, \\ b_k &= S^{(k)} - S^{(k-1)}. \end{aligned} \tag{2.16}$$

By construction, the kth iterate $S^{(k)}$ is given by the sum of $k+1$ terms of the power series

$$S_k(x) = \sum_{r=0}^{k} b_r x^r, \tag{2.17}$$

evaluated at $x = 1$:

$$S^{(k)} = S_k(1). \tag{2.18}$$

A Padé approximant to the polynomial $S_k(x)$ of order k is a rational function (ratio of polynomials)

$$[L/M] = \frac{P_L(x)}{Q_M(x)} \quad (L+M=k), \tag{2.19}$$

whose coefficients are chosen such that the first k terms of its Maclaurin expansion coincide with $S_k(x)$. Techniques for evaluating the coefficients in $P_L(x)$ and $Q_M(x)$, discussions of the use of $[L/M]$ as a more accurate representative of the function approximated by S_k, and analyses of convergence will be found in textbooks on Padé theory.[9] We use the Wynn[10] algorithm to generate directly the approximants $[L/L]$ and $[L+1/L]$ for $x = 1$. The algorithm described by Patry and Gupta[11] is a reasonably stable method of computing the coefficients of the polynomials P and Q in Eq. (2.19).

Numerical studies in Sec. III will show that sequences of Padé approximants to $S_k(x)$ such as

$$\begin{matrix} [0/0] & [1/0] & [1/1] & [2/1] & [2/2] & \ldots \\ (k=0) & (k=1) & (k=2) & (k=3) & (k=4) & \ldots \end{matrix}, \tag{2.20}$$

evaluated of course at $x = 1$, accelerate the convergence of the original sequence (2.14) when it converges, and continue to converge rapidly under many circumstances in which the original sequence diverges, providing that the sequence was generated by either block or sequential iteration. It should be noted, however, that we have obtained only converged S-matrix elements; we do not obtain improved wave functions so our results cannot be used as input to coupled-channels Born-approximation calculations.

The Padé approximants have a very useful feature if the original sequence (2.14) was generated by block iteration. In this case the successive differences b_k are proportional to the kth power of the coupling potential. If an overall coupling parameter Λ is factored out of the coupling potential [$U \to \Lambda\tilde{U}$ in Eq. (2.1)], we can regard x in Eqs. (2.17) and (2.19) as

$$x = \Lambda/\Lambda_0, \tag{2.21}$$

where Λ_0 is the value of Λ for which the sequence (2.14) was generated. Evaluating Eqs. (2.17) or (2.19) for values of x different from 1 then gives the S-matrix element as a function of Λ. With this method the S-matrix elements can easily be found for other values of Λ once they have been calculated for any single value. This could be of practical utility if it were desired to determine a deformation parameter by fitting computed cross sections to data; when the coupling potential is derived from a first order collective model of a single multipolarity with the equal nuclear and Coulomb deformations, the overall coupling parameter Λ may be identified as the deformation parameter β.

As is evident from Eq. (2.12), the successive differences b_k computed by sequential iteration are not proportional to a single power of the coupling potential. Thus in this case we cannot use Eq. (2.19) with $x \neq 1$ to evaluate S as a function of Λ. One must therefore choose between the more rapid convergence of the sequential iteration method and the advantage of being able to compute S simultaneously for more than one value of Λ.

C. Method of moments

The method of moments[12] is an iterative technique for the solution of the integral equivalent of the coupled differential equations (2.1); a finite set of basis functions is defined iteratively and at each stage the integral equations are solved in the truncated basis constructed up to that point. The linearly independent basis functions used are in fact differences of the functions $R_\alpha^{(i)}$ generated by block iteration; the basis functions are defined by

$$u_\alpha^{(0)} = R_\alpha^{(0)} = \delta_{\alpha\alpha_0} f_{\alpha_0}, \tag{2.22}$$

$$u_\alpha^{(i)} = R_\alpha^{(i)} - R_\alpha^{(i-1)} \quad (i = 1, \ldots, k). \tag{2.23}$$

These basis functions are defined only on the interval $0 \leq r \leq R_N$, where R_N has previously been

defined as the boundary of the interior region.

We introduce the integral operator

$$K_{\alpha\beta}(r,r') = D_\alpha^{-1}(r,r')U_{\alpha\beta}(r'), \quad 0 \le r,\ r' \le R \tag{2.24}$$

where D_α^{-1} designates the (outgoing-wave) Green's function associated with the differential operator D_α of Eq. (2.1). The successive basis functions are related by application of the operator K:

$$u_\alpha^{(i)}(r) = \sum_\beta \int_0^R dr' K_{\alpha\beta}(r,r') u_\beta^{(i-1)}(r'). \tag{2.25}$$

For all potentials of interest here the scalar products

$$\langle u^{(j)} | u^{(i)} \rangle = \sum_\alpha \int_0^R dr\, [u_\alpha^{(j)}(r)]^* u_\alpha^{(i)}(r) \tag{2.26}$$

of the basis functions are finite. [$u^{(i)}$ is a vector with N components $u_\alpha^{(i)}$.]

We let $H^{(k-1)}$ be the space spanned by the k vectors $u^{(0)}, u^{(1)}, \ldots, u^{(k-1)}$ and let $P^{(k-1)}$ be a projection operator onto it. We determine a vector $\hat{R}^{(k)}$ in $H^{(k-1)}$ that is the solution of the integral equivalent of the coupled equations (2.1) restricted to the space $H^{(k-1)}$:

$$\hat{R}_\alpha^{(k)}(r) = \delta_{\alpha\alpha_0} f_{\alpha_0}(r) + \sum_\beta \int_0^R dr' K_{\alpha\beta}^{(k-1)}(r,r') \hat{R}_\beta^{(k)}(r'), \tag{2.27}$$

where

$$K^{(k-1)} = P^{(k-1)} K P^{(k-1)}. \tag{2.28}$$

If we express $\hat{R}^{(k)}$ as a linear combination of the basis functions that span $H^{(k-1)}$,

$$\hat{R}^{(k)} = \sum_{i=0}^{k-1} a_i u^{(i)}, \tag{2.29}$$

and substitute in Eq. (2.27), we obtain a set of linear equations for the expansion coefficients:

$$\sum_{i=0}^{k-1} a_i u^{(i)}(r) = u^{(0)}(r) + \sum_{i=0}^{k-2} a_i u^{(i+1)}(r) + a_{k-1} P^{(k-1)} u^{(k)}(r), \tag{2.30}$$

where we have made use of

$$P^{(k)} u^{(i)} = u^{(i)} \quad (i = 0, \ldots, k-1). \tag{2.31}$$

For the last term of Eq. (2.30), we write

$$P^{(k-1)} u^{(k)} = \sum_{i=0}^{k-1} b_i^{(k)} u^{(i)}, \tag{2.32}$$

where the $b_i^{(k)}$ satisfy the linear equations

$$\sum_{j=0}^{k-1} \langle u^{(i)} | u^{(j)} \rangle b_j^{(k)} = \langle u^{(i)} | u^{(k)} \rangle \quad (i = 0, \ldots, k-1). \tag{2.33}$$

Inserting Eqs. (2.32) in Eq. (2.30) and equating the coefficients of each $u_\alpha^{(i)}$, we obtain

$$a_0 = 1 - b_0/Q \tag{2.34}$$

and

$$a_i = a_{i-1} - b_i/Q \quad (i = 1, \ldots, k-1), \tag{2.35}$$

where

$$Q = 1 + \sum_{i=0}^{k-1} b_i. \tag{2.36}$$

The approximation $\hat{S}_{\alpha\alpha_0}^{(k)}$ to the S matrix at the kth iteration is obtained by substituting the approximate wave function $\hat{R}^{(k)}$ in the integral identity (2.7). Equation (2.25) may be rewritten in differential form:

$$D_\alpha u_\alpha^{(i+1)} = \sum_\beta U_{\alpha\beta} u_\beta^{(i)}. \tag{2.37}$$

Substituting the expansion (2.29) in Eq. (2.7) and using Eq. (2.37), we find

$$\hat{S}_{\alpha\alpha_0}^{(k)} = \delta_{\alpha\alpha_0} S_{\alpha_0} - \frac{2i}{(k_\alpha k_{\alpha_0})^{1/2}} \times \sum_{i=0}^{k-1} a_i \int_0^R dr f_\alpha(r) D_\alpha(r) u_\alpha^{(i+1)}(r). \tag{2.38}$$

Integration by parts and the Wronskian relations for the Coulomb functions then give the result

$$\hat{S}_{\alpha\alpha_0}^{(k)} = \delta_{\alpha\alpha_0} S_{\alpha_0} + \sum_{i=0}^{k-1} a_i (S_{\alpha\alpha_0}^{(i+1)} - S_{\alpha\alpha_0}^{(i)}), \tag{2.39}$$

where $S_{\alpha\alpha_0}^{(i)}$ is the S-matrix element associated with the asymptotic form of $R_\alpha^{(i)}$ by Eq. (2.4). Thus it is not necessary to evaluate the integral in Eq. (2.7) because the $S_{\alpha\alpha_0}^{(i)}$ are available from the construction of the $R_\alpha^{(i)}$.

It should be noted that the improved wave functions $\hat{R}_\alpha^{(k)}$ and the associated S-matrix elements $\hat{S}_{\alpha\alpha_0}^{(k)}$ are not used in the next iteration of the method of moments. Rather $R_\alpha^{(k+1)}$ and $S_{\alpha\alpha_0}^{(k+1)}$ are generated by block iteration from $R_\alpha^{(k)}$ and the coupled integral equations (2.27) solved in the resulting larger space. It has been proved that the iterative process of the moment method converges for any local potential, regardless of its strength.[4]

The S-matrix elements obtained from the method of moments are rational functions of the coupling strength. If we factor out an overall coupling strength Λ from $U_{\alpha\beta}$, it is clear that $u^{(i)}$ is proportional to Λ^i. Hence, as was the case for block iteration with Padé acceleration, given the $\hat{S}_{\alpha\alpha_0}^{(k)}$ for a specific Λ, it is easy to generate S matrices for other values of Λ.

D. A simplified variant of the Sasakawa method

The original Sasakawa[6] iterative scheme has

been shown[7] to converge for a class of potentials that includes all those of interest here: however, the multichannel generalization[8] of the Sasakawa method involves too much computational labor per iteration to be useful. Austern[5] and Soper[8] have studied a modification of the Sasakawa method that reduces the amount of computation to a reasonable level. The modified iteration scheme, however, does not have any of the convergence guarantees of the original method.

The basic idea is to modify the coefficient of the outgoing part of the radial wave functions obtained by solution of the inhomogeneous equations (2.10) such that at each iteration the modified radial functions $\hat{R}_\alpha^{(k)}$ and S-matrix elements $\hat{S}_{\alpha\alpha_0}^{(k)}$ satisfy the integral (2.7). In block iteration, this relation holds only after a converged solution has been obtained. Suppose, then, that a set of radial wave functions $\hat{R}_\alpha^{(k-1)}$ has been generated by $(k-1)$ iterative steps. The kth step of the Austern-Sasakawa procedure is then carried out as follows.

The radial functions $\hat{R}_\alpha^{(k-1)}$ are substituted in the right-hand side of Eqs. (2.10) and the resulting inhomogeneous equations solved for a new set of approximations $\hat{R}_\alpha^{(k)}$ and $\hat{S}_{\alpha\alpha_0}^{(k)}$. This portion of the calculation is identical to the kth step of block iteration. Auxiliary functions $J_\alpha^{(k)}$ are then defined by

$$J_\alpha^{(k)}(r)=\frac{R_\alpha^{(k)}(r)-\delta_{\alpha\alpha_0}f_\alpha(r)}{S_{\alpha\alpha_0}^{(k)}-\delta_{\alpha\alpha_0}S_\alpha}. \tag{2.40}$$

Corrected radial wave functions $\hat{R}_\alpha^{(k)}$ are given by

$$R_\alpha^{(k)}=\delta_{\alpha\alpha_0}f_{\alpha_0}(r)+(\hat{S}_{\alpha\alpha_0}^{(k)}-\delta_{\alpha\alpha_0}S_{\alpha_0})J_\alpha^{(k)}, \tag{2.41}$$

where the S-matrix elements $\hat{S}_{\alpha\alpha_0}^{(k)}$ are to be determined from the integral relation (2.7). Substitution of (2.41) in (2.7) yields the set of inhomogeneous linear equations

$$\hat{S}_{\alpha\alpha_0}^{(k)}=\delta_{\alpha\alpha_0}S_{\alpha_0}-\frac{2i}{(k_\alpha k_{\alpha_0})^{1/2}}\int f_\alpha U_{\alpha\alpha_0}f_{\alpha_0}$$
$$-\frac{2i}{(k_\alpha k_{\alpha_0})^{1/2}}\sum_\beta\int f_\alpha U_{\alpha\beta}J_\beta(\hat{S}_{\beta\alpha_0}^{(k)}-\delta_{\beta\alpha_0}S_{\alpha_0}) \tag{2.42}$$

for the S-matrix elements. The solutions then determine the modified radial functions $\hat{R}_\alpha^{(k)}$ with the help of Eqs. (2.41).

E. Computer requirements

A complete comparison of the relative efficiency of the various methods must involve not only the number of iterations needed to achieve a desired accuracy, but also the time and storage requirements for an iteration of each technique. The convergence rates of the various iterative schemes are compared in Sec. III. Here we discuss the computer time and storage requirements. We have identified those parts of the calculations that demand the most computing time and storage and estimated the time and storage that would be needed by efficient programs implementing each method. The time required to compute Coulomb wave functions (or coupled-channels Coulomb wave functions) has not been included in these estimates.

Storage requirements are given in terms of floating point (real) numbers or "words." A complex number requires two such words. We have found that single precision (32 bits) on IBM 370 computers is adequate for all of the large arrays used in these calculations. Modern large-scale computers have the ability to overlap the processing of several operations such as accessing memory, decoding instructions, computing subscript quantities and floating-point operations. For this reason the execution times of large scientific programs depend most heavily on the number of floating-point operations (FLOP) that must be made—auxiliary computations such as subscript evaluations may be ignored. We present timing estimates in terms of the number of floating-point operations; in calculations similar to the ones described here the CDC 7600 and IBM 370/195 computers are capable of about 5×10^6 FLOP/sec, the CRAY-I computer about 50×10^6 FLOP/sec.

In the estimates we assume that the Numerov method as described in Ref. 2 is used to generate all radial functions $R_\alpha^{(k)}$. This method computes the wave function on a grid of equally spaced coordinate values and requires the potentials on the same grid. The integration starts at some value of r (not necessarily at $r=0$) for which the wave function is negligible. If the grid contains M points, then the Numerov method for inhomogeneous equations may be executed in $20M$ floating-point operations.

There are N^2 complex potential functions for N coupled equations and each of these is required at M grid points. Clearly it is impractical to store such a three-dimensional array for large N or M. Instead we will make the following assumptions that seem reasonable for heavy-ion calculations. The optical potential is the same for all channels. In addition a separate array containing r^{-2} is stored to allow rapid computation of the centrifugal term in the kinetic energy. The coupling potentials can be expressed in the form

$$U_{\alpha\beta}(r)=\sum_i X_{\alpha\beta}^{(i)}v_i(r), \tag{2.43}$$

where $X_{\alpha\beta}^{(i)}$ is independent of r and contains all

angular-momentum-coupling factors while $v_i(r)$ is independent of the labels α and β. There are separate v_i for each distinct function of r (each multipolarity and order of coupling) appearing in $U_{\alpha\beta}$. Since there are typically only a few v_i, separate storage of the $X^{(i)}_{\alpha\beta}$ and the $v_i(r)$ allows the potentials to be saved in a reasonable amount of core. We use N_v to designate the number of different v_i that must be stored. The $X^{(i)}_{\alpha\beta}$ may be chosen to be real. In many problems each R_α will be coupled to only a few of the N functions R_β and $X^{(i)}_{\alpha\beta}$ may have the form of a band matrix. We use N_c to designate the average number of couplings per channel basis state. Because the best way to store the matrices $X^{(i)}_{\alpha\beta}$ depends on whether or not they are band matrices, we do not include their size in the storage estimates that follow.

Table I presents our estimates of the storage and time requirement of the various iterative techniques. The first part of the table summarizes the symbols that are used in the estimates and gives their values for two extreme computations. The first is a simple two-channel calculation involving ^{16}O and ^{44}Ca. The second is sub-Coulomb $E2$ excitation of ^{154}Sm by 900 MeV ^{208}Pb ions including states up to $J=20^+$ in the ground-state rotational band. We have not yet attempted a calculation as large as this one. The wavelength for the reaction is 0.156 fm, so the 1500 steps ($M=1500$) indicated in the table correspond to ten steps per wavelength starting from 11 fm and going out to 35 fm, which is a resonable matching radius if the coupled-channels Coulomb functions are used.

The second part of Table I presents the core and time estimates as functions of the relevant parameters and for the two reactions. The time estimates are in terms of FLOP/iteration. It can be seen that an iteration of the Austern-Sasakawa method is two or three times slower than an iteration of the block method. The method of moments requires less additional time but needs much more storage to save the wave functions at each iteration. The last line of the table shows the requirements of the traditional method of solving the coupled equations (construction of N linearly independent sets of solutions of the N coupled equations). Because the time for this method varies as N^3, a solution for the second example requires the equivalent of 2100 block iterations.

Griffen and Koshel have suggested expanding the R_α in plane waves as a method of solving the inhomogeneous differential equations. Because it takes many fewer expansion coefficients than values on a coordinate grid to represent each R_α with adequate accuracy, the plane-wave method significantly reduces the storage requirements of the method of moments. Both the core and time requirements for the plane-wave method depend upon the number of plane waves needed to represent the R_α. Plane-wave matrix elements of the potentials and operators such as D_α must be computed and stored. The solution of the inhomogeneous equation is then reduced to the solution of a set of simultaneous equations; the time for this is proportional to the cube of the number of plane

TABLE I. Core and time estimates for the methods discussed in the text. The first part gives the symbols used and reasonable values for two calculations. (1) ^{16}O + ^{44}Ca at 60 MeV using the 0^+ and 2^+ states of ^{44}Ca, (2) ^{208}Pb + ^{154}Sm at 900 MeV using the 0^+, 2^+, ..., 20^+ ground-state rotational band of ^{154}Sm with quadrupole coupling. Core estimates are in floating-point words, time estimates in floating-point operations (FLOP).

Symbol	Meaning	Values Example 1	Values Example 2
N	Number of coupled equations	4	121
M	Number of Numerov grid points	200	1500
N_v	Number of $v_i(r)$	1	1
N_c	Number of couplings per equation	4	9
n	Number of iterations	5	5

Method	Core (Floating words)	Time/Iteration (FLOP)	Example 1 Core 10^3 words	Example 1 time 10^3 FLOP	Example 2 Core 10^6 words	Example 2 time 10^6 FLOP
Block	$M(4N+2N_v+3)$	$MN[30+N_v(4N_c+6)]$	5.0	41.6	0.74	13.4
Sequential	$M(4N+2N_v+5)$	$MN[30+N_v(4N_c+6)]$	5.0	41.6	0.74	13.4
Austern-Sasakawa	$M(6N+2N_v+3)+2N^2$	$MN[36+N_v(14N_c+12)]+\frac{8}{3}N^3$	6.2	84	1.13	53.9
Moments	$M[(2n+4)N+2N_v+3]$	$MN[40+4n+N_v(4N_c+6)]$	11.4	66.6	2.13	18.9
Conventional	$M(2N_v+3)+12N^2[+2N^2M]$ [a]	$M(11N^3+4N^2)[+8MN]$ [a]	1.6 [b]	154 [b]	0.19 [b]	29 000.0 [b]

[a] Required only if wave functions needed.
[b] Wave function computation not included.

waves. We have made a few studies of the number of plane waves needed and conclude that for example 1, 30 plane waves are necessary,[13] 60 or more for example 2. In both cases the plane-wave expansion technique requires somewhat more storage and more than thrice the time than the grid method to construct the radial functions $R_\alpha^{(n)}$.

III. COMPARISON OF ITERATIVE METHODS

We have used a rather simple coupled-channels problem to assess the convergence rates of the iterative techniques described in Sec. II. The two coupled channels are $^{16}O + {}^{44}Ca$ (g.s.) and $^{16}O + {}^{44}Ca$ (2^+, 1.156 MeV). Calculations were made for a bombarding energy of 60 MeV. The optical potential is of the Woods-Saxon form with identical real and imaginary radial dependence; the potential parameters are

$$V = 110 \text{ MeV}, \quad W = 20 \text{ MeV},$$
$$r_0 = 1.2 \text{ fm}, \quad a = 0.5 \text{ fm}, \tag{3.1}$$
$$r_{c_0} = 1.2 \text{ fm},$$

where V and W are respectively the real and imaginary well depths, r_0 is the radius parameter, a is the diffuseness, and r_{c_0} is the Coulomb radius parameter. The potential radii (both Coulomb and nuclear) are related to the radius parameters by

$$R' = r_0(A_P^{1/3} + A_T^{1/3}), \tag{3.2}$$

where A_P and A_T are the projectile and target atomic weights. The rotational model [Eq. (2.10) of Ref. 1] was used for $U_{\alpha\beta}$. In the calculations reported here only nuclear coupling was considered ($\beta_c = 0$). This represents a stringent test of the methods of solution since the sharply peaked nuclear coupling results in significantly distorted wave functions. Coulomb coupling reduces the distortion and the number of iterations necessary to achieve a given accuracy. Nuclear reorientation effects and the diagonal elements of $U_{\alpha\beta}$ are included in the calculations. Most of the calculations were made for $J = 30$ (a near-grazing partial wave) for which the elastic S matrix has the magnitude $|S^{J=30}_{30,0^+;\,30,0^+}| = 0.46$.

Tables II and III compare the rate of convergence of the magnitude of one of the inelastic S-matrix elements ($|S^{J=30}_{30,2^+;\,30,0^+}|$) for the various techniques. Table II is for a physically reasonable deformation parameter ($\beta = 0.25$) while Table III is for a much larger value ($\beta = 0.4$). The calculation for this unrealistic deformation value is of course much harder; it is of interest as a simulation of realistic calculations involving the strongly deformed rare-earth nuclei.

The tables show the convergence as a function of iteration number k; in comparing the different techniques we must take into account the time estimates given in Table I. In the Padé columns the $[M/M]$ Padé estimate is given for the even-numbered iterations, the $[M/M-1]$ estimate for the odd, as illustrated in sequence (2.17).

Table II shows that with the possible exception

TABLE II. Convergence properties of the modulus of the inelastic S-matrix element $|S^{30^+}_{30,2^+;30,0^+}|$, as a function of iteration number k, for the reaction $^{44}Ca(^{16}O,{}^{16}O)^{44}Ca(2^+1.156 \text{ MeV})E_{\text{Lab}} = 60$ MeV. The numerical techniques are described in Sec. II. The potentials used are given in Sec. III. The nuclear deformation is $\beta = 0.25$.

k	Sequential	Sequential and Padé	Block	Block and Padé	Method of moments	Austern-Sasakawa
1	0.1269	0.1269	0.1695	0.1695	0.1695	0.1258
2	0.1611	0.1593	0.1472	0.1487	0.1436	0.1478
3	0.1492	0.1484	0.1530	0.1594	0.1611	0.1487
4	0.1467	0.1481	0.1665	0.1510	0.1481	0.1474
5	0.14802	0.14793	0.1340	0.1475	0.1501	0.1479
6	0.14806	0.14797	0.1514	0.1478	0.1479	0.1481
7	0.14796	0.147971	0.1535	0.14791	0.14788	0.14790
8	0.14798	0.14795	0.1384	0.14795	0.14807	0.14798
9	0.147976	0.14795	0.1549	0.14795	0.14798	0.14792
10	0.147974		0.1476	0.14794	0.14796	0.14797
11	0.14795		0.1433	0.14796	0.147976	0.14798
12	0.14795		0.1546	0.147971	0.147976	0.14793
13			0.1438	0.14793		0.14796
14			0.1474	0.147976		0.14796
15			0.1525	0.147976		0.14795
16			0.1429			
17			0.1502			
18			0.1499			
19			0.1439			
20			0.1514			

TABLE III. Convergence properties of the modulus of the inelastic S-matrix element $|S^{30^+}_{30,2^+;30,0^+}|$ for the reaction and potentials of Table II with $\beta = 0.4$.

k	Sequential	Sequential and Padé	Block	Block and Padé	Method of moments	Austern-Sasakawa
1	0.1634	0.16 32	0.2713	0.27 13	0.27 13	0.1561
2	0.2906	0.23 60	0.2157	0.22 10	0.21 03	0.2050
3	0.2540	0.20 78	0.2921	0.25 36	0.26 21	0.2067
4	0.1448	0.20 95	0.3390	0.22 20	0.21 28	0.1987
5	0.2035	0.20 81	0.0222	0.20 47	0.22 47	0.2075
6	0.2494	0.20 70	0.4046	0.20 41	0.20 54	0.2098
7	0.2125	0.20 72	0.4645	0.20 58	0.20 93	0.2043
8	0.1747	0.20 713	0.3390	0.20 63	0.20 66	0.2077
9	0.2156	0.20 717	0.9398	0.20 63	0.20 64	0.2056
10	0.2293	0.20 7173	0.9914	0.20 59	0.20 716	0.2113
11	0.1971	0.20 7170	1.481	0.20 65	0.20 716	0.2092
12	0.1950	0.20 7175	2.501	0.20 69	0.20 717	0.1995
13	0.2182	0.20 7175	3.296	0.20 69	0.20 718	0.2116
14	0.2134		5.290	0.20 713	0.20 717	0.2080
15	0.1980		8.068	0.20 717	0.20 7176	0.2013
16	0.2054		11.79	0.20 719	0.20 7175	0.2146
17	0.2142		18.26	0.20 7179	0.20 7175	0.2042
18	0.2068		27.27	0.20 7175	0.20 7175	0.2036
19	0.2023		40.80	0.20 7176	0.20 7176	0.2156
20	0.2088		61.64	0.20 7175	0.20 7175	0.2001

of the unmodified block method, all the methods converge for $\beta = 0.25$. At $\beta = 0.4$ (Table III) both the block and Austern-Sasakawa methods fail to converge and the sequential method is converging very slowly (we have continued the calculations to 40 iterations to verify these statements).

Sequential iteration with Padé acceleration is clearly the most rapidly convergent method for $\beta = 0.4$; it achieves an accuracy of 0.5% in five iterations while the method of moments requires eight and block iteration with Padé acceleration requires 11 iterations to achieve the same accuracy. For $\beta = 0.25$ both sequential iteration with Padé and Austern-Sasakwa require only three iterations to achieve 0.5% accuracy; block iteration with Padé and unaccelerated sequential require five iterations and the method of moments needs six iterations. For these cases, and all others studied, Padé approximants do not increase the convergence rates of either the method of moments or the Austern-Sasakawa method.

Although the Austern-Sasakawa technique converged rapidly for $\beta = 0.25$, the divergence for $\beta = 0.4$ together with the substantial computer storage and time requirements suggests that this method is not competitive for heavy-ion coupled-channels calculations.

As was described in Sec. II, both block iteration with Padé acceleration and the method of moments allow straightforward evaluation of S-matrix elements as a function of β, once they are computed for a single value of β. Figures 1 and 2 show the resulting curves for block iteration with Padé acceleration and the method of moments, respectively. The curves are labeled with the number of iterations that were used to generate them. In both cases the first iteration is just the first-order Born result. For the first nine iterations, the block method is clearly superior to the method of

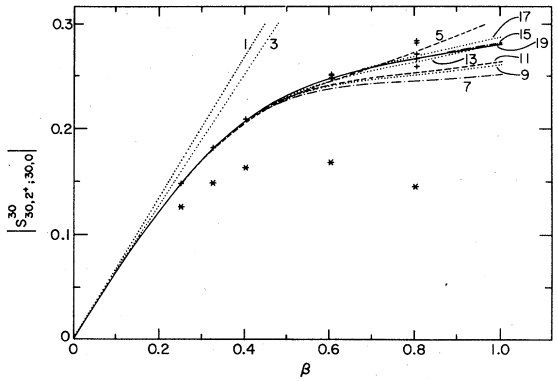

FIG. 1. The modulus of the inelastic S-matrix element $|S^{30}_{30,2^+;30,0}|$, plotted as a function of the nuclear deformation parameter, for the reaction ^{44}Ca(^{16}O, ^{16}O)^{44}Ca(2^+, 1.156 MeV) at $E_{LAB} = 60$ MeV. The lines represent the results of block iteration with Padé approximants and are labeled by the number of iterations k. The stars represent the values obtained from sequential iteration and Padé approximants for $k = 1$. The crosses give the corresponding results obtained for k ranging from 3 to 11. The potential parameters used in this calculation are listed in Sec. III.

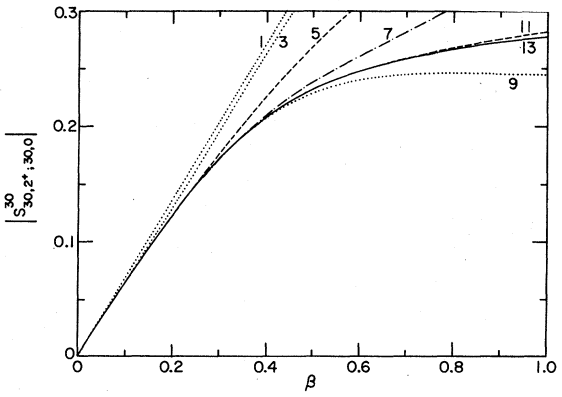

FIG. 2. The modulus of the inelastic S-matrix element shown in Fig. 1, for various numbers of iterations obtained by the method of moments.

moments. However, for $\beta > 0.6$ the convergence of block iteration with Padé acceleration significantly slows down for iterations 11 to 17 and the 19th iteration is only as good as the 11th iteration of the method of moments. This wandering of the Padé accelerant appears to be an intrinsic feature of the Padé method because several different ways of evaluating the Padé approximants (the Wynn and epsilon algorithms,[10] Patry and Gupta's method,[11] and matrix inversion[9]) produce the same results. The method of moments does not seem to exhibit this phenomenon of a temporary interruption in its march towards a fully converged result.

The points in Fig. 1 show the results of separate Padé-accelerated sequential-iteration calculations for five values of β. It is obvious that if one is not interested in results for more than one value of β, this method is far more rapidly convergent than block iteration with Padé or the method of moments.

We have also tried these six methods for the $^{16}O + ^{44}Ca$ reaction for $J = 10$ with similar conclusions. The sequential-iteration method with Padé acceleration has also been used by us for many other two-channel heavy-ion reactions such as $^{136}Xe + ^{208}Pb$ and $^{18}O + ^{184}W$. In an attempt to simulate a multichannel calculation we considered the excitation of a 16^+ state by a $\lambda = 16$ transition with $\beta_{16} = 0.5$ for which the Born series rapidly diverged; 0.1% accuracy was achieved in only nine iterations of the Padé-accelerated sequential method. Except for some extraordinarily large unphysical values of β, this method has always been found to converge, usually to 0.1% accuracy in fewer than seven iterations.

IV. INWARD-OUTWARD ITERATION METHODS

In the first paper of this series, we used the Alder-Pauli[2] transformation to solve for the Coulomb part of heavy-ion inelastic scattering. The channel wave functions in the exterior region are expressed as products of Coulomb functions and modulating amplitudes and the coupled equations for the modulating amplitudes are reduced to first order and shown to be capable of accurate solution in first Born approximation; this latter step permits the use of recursion relations in angular momentum that in turn eliminate the need to integrate explicitly in all but a few partial waves. Iterative techniques for solution of the radial equations in the interior region are the topic of the present study.

Alder, Roesel, and Morf[14] and Ichimura *et al.*[15] have proposed a different strategy. The Alder-Pauli transformation is to be used over the entire range of r values; the distinction between interior and exterior regions disappears. This involves finding not only incoming and outgoing solutions, but also the S-matrix elements. Alder *et al.* approach this combined problem of solving the coupled equations and imposing appropriate boundary conditions by an iterative procedure. A first estimate of the S-matrix elements is made and the coupled equations are integrated inwards from infinity; regularity is imposed at small r and the coupled equations integrated outwards to obtain an improved estimate of the pertinent S-matrix elements. The whole process is iterated until adequate accuracy has been achieved in the S-matrix elements. Recently Tolsma[16] has studied a variant of this procedure in which the asymptotic Coulomb functions of the Alder-Pauli transformation are replaced by Airy functions; the coupled equations for the modulating functions are solved by inward-outward iteration.

Tolsma considers Coulomb excitation only and presents impressive results, including a computation of excitation of rotational bands in deformed nuclei up to $I = 24^+$; these are by far the largest quantal Coulomb excitation calculations ever carried out. There is, however, one aspect of Tolsma's work on which we wish to comment. He compares inward-outward iteration with sequential iteration as a method of solution of the equations for the modulating amplitudes and finds that sequential iteration diverges for some cases of interest. He concludes that inward-outward integration is superior. We have shown, however, that Padé acceleration (which Tolsma does not consider) eliminates convergence problems when using sequential iteration to solve the coupled radial equations in the interior region. It appears that Tolsma's argument as to the relative merits of inward-outward and sequential iteration is incomplete.

We have not made detailed studies of the relative

efficiency of inward-outward iteration and the methods discussed here. However, Tolsma implies that his method is some 30 times faster than the conventional method, for example 2 of Table I. As can be seen from the table, ten sequential iterations with Padé acceleration (which should be adequate to achieve convergence) should be some 200 times faster than the conventional method for the same problem.

V. CONCLUSIONS

Of the iterative methods considered, sequential iteration with Padé acceleration is the most reliable and rapidly convergent; typically it gives 0.5% accuracy in three or four iterations. In addition it requires considerably less storage and time per iteration than the more complicated Austern-Sasakawa and moment methods. Its principal defect in the form we have discussed is that the Padé approximants are used to improve the convergence of the S-matrix elements only. For calculations requiring converged wave functions it would be possible to apply Padé approximants point by point to each set of iterated channel wave functions. Although this would substantially increase the computer storage required, it will usually be possible to avoid storing every iterated wave function in each channel; thus even with point-by-point Padé approximation of the wave functions, sequential iteration should in practice require considerably less storage than the method of moments. Other schemes for computing the wave functions once accurate S-matrix elements are known might also be considered, but it seems to us that the Padé approximants will prove most useful when it is not necessary to obtain the scattering wave functions.

A hypothetical calculation considered in this paper is excitation of the ground-state rotational band of ^{154}Sm up to the 20^+ level by a 900 MeV ^{208}Pb projectile. We would expect sequential iteration with Padé acceleration to complete this calculation in about 0.005 of the time required by the conventional method of solving the N equations N times. This tremendous increase in speed makes such calculations fully feasible on present computers.

ACKNOWLEDGMENTS

We are indebted to Dr. Fritz Coester for many helpful comments, criticisms, and suggestions. This work was supported by the U.S. Department of Energy.

[1]M. Rhoades-Brown, M. H. Macfarlane, and S. C. Pieper, Phys. Rev. C 21, 2417 (1980).
[2]K. Alder and H. C. Pauli, Nucl. Phys. 128, 1931 (1969).
[3]J. Raynal, *Computing As a Language of Physics* (IAEA, Vienna, 1972), p. 281.
[4]P. J. Griffin and R. D. Koshel, Ann. Phys., to be published.
[5]N. Austern, Phys. Rev. 188, 1595 (1969).
[6]T. Sasakawa, Prog. Theor. Phys. Suppl. 27, 1 (1963).
[7]F. Coester, Phys. Rev. C 3, 525 (1970).
[8]P. Soper, Phys. Rev. C 10, 1282 (1974).
[9]G. Baker, *Essentials of Padê Approximants* (Academic, New York, 1975).
[10]P. Wynn, Numer. Math. 8, 264 (1966).
[11]J. Patry and S. Gupta, EIR-BERICHT NR247 EIDG. Institut für Reaktorforschung, Würenlingen, Switzerland, 1973.
[12]Our description of the method of moments parallels that of Ref. 4. However, our notation, in particular the meaning of the superscripts on $P^{(n)}$ and $H^{(n)}$, is somewhat different from that of Ref. 4.
[13]R. D. Koshel (private communication) also found 30 terms are necessary.
[14]K. Alder, F. Roesel, and R. Morf, Nucl. Phys. A284, 145 (1977).
[15]M. Ichimura, M. Igaroshi, S. Landowne, C. H. Dasso, B. S. Nilsson, R. A. Broglia, and A. Winther, Phys. Lett. 67B, 129 (1977).
[16]L. D. Tolsma, Phys. Rev. C 20, 592 (1979).