Statement of Approximate Locality

(3) The factorization of the probability for two separate events Eq. (1)

$$P(b,g_x \leftarrow a,f_x) \xrightarrow[|x|\to\infty]{} P(b \leftarrow a)P(g \leftarrow f).$$

This was strengthened in Eq. (10) by replacing the state f_x by $(f_x+f'_{x'})$ and g_x by $(g_x+g'_{x'})$, and requiring that the corresponding limit hold as $|x|$ and $|x'| \to \infty$ [uniformly with respect to $(x-x')$ of course].

(4) The analogous factorization for three separate experiments as in Eq. (13).

Superselection Rules

(5) Superselection rules defined by discrete additive quantum numbers; namely, charge, baryon, and lepton numbers.[22]

[22] In fact the method of Sec. IV can accommodate any number of quantum numbers of this kind, including those with infinitely many eigenvalues, such as charge, and those with a finite number of eigenvalues, such as the separation of integral and half-odd-integral angular momenta.

These assumptions led first to factorization of S-matrix elements and thence, using the argument of Wichmann and Crichton, to the momentum-space equations, whose final form is shown in Fig. 3 and Eq. (20). While this form may differ from the usual one shown in Fig. 1—a difference which would show up in interference experiments between states of different particle type—nonetheless the unitarity equations for the connected parts take precisely the usual form assumed in analytic S-matrix theory.

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Application of the Padé Approximant to Scattering Theory†

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The Padé approximant is shown to yield exactly unitary S matrices in scattering theory. The method is used to construct a unitary S matrix for n-d scattering above the threshold for inelastic scattering. Thus the effect of inelastic scattering on elastic-scattering total cross sections and angular distributions is calculated. No cusps are found at the threshold.

I. INTRODUCTION

THE Padé approximant[1] has been applied to summing series which occur in calculations based on the Ising and Heisenberg models of various types of critical phenomena.[2] The Padé approximant may also be applied to the Born series which occur in scattering theory; recently Tani[3] has made a study of this application.

In this paper we show that the Padé approximant method may be used to construct exactly unitary S matrices. In problems in which states with more than two free particles are energetically possible (the example we are concerned with is n-d scattering above the threshold for inelastic scattering; however, there are many others of great interest, for example, nucleon-nucleon or pion-nucleon scattering above the threshold for pion production) the problem of constructing unitary S matrices has not been satisfactorily solved previously.

In calculations of n-d elastic scattering based on the no-distortion approximation,[4] inelastic scattering is ignored even above the threshold for inelastic scattering. Because of this neglect of inelastic scattering, the matrix elements for transitions between states in which three particles are free are not required because in the no-distortion approximation three-body states are precisely what are left out. Our work represents an attempt to go beyond the no-distortion approximation. In calculations of n-d inelastic cross sections based on

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[1] For a review, see G. A. Baker, Jr., in *Advances in Theoretical Physics*, edited by K. A. Brueckner (Academic Press Inc., New York, 1965), Vol. 1.
[2] See the surveys of M. Fisher and C. Domb in the Proceedings of the Conference on Phenomena in the Neighborhood of Critical Points, Washington, D. C., 1965 (unpublished).
[3] S. Tani, Phys. Rev. **139**, B1011 (1965).
[4] See, for example, R. S. Christian and J. L. Gammel, Phys. Rev. **91**, 100 (1953).

the Born approximation or some modification of it,[5] the S matrix (which must describe elastic and inelastic processes simultaneously and also transitions between states in which three particles are free) calculated is not unitary. The consequences of this fact have never been assessed.

In using the Padé approximant to construct an exactly unitary S matrix, we so arrange our work that in the limit of vanishing inelastic scattering our result for the elastic scattering agrees with Christian and Gammel's result; in particular, below threshold for inelastic scattering we obtain Christian and Gammel's result. Thus we are able to estimate the effect of possible inelastic scattering on the elastic scattering differential cross sections. We do not find cusps at the threshold for inelastic scattering in the n-d total cross section or in the differential cross section at a fixed angle as a function of the center-of-mass energy. We obtain a new result for the inelastic cross section (which includes the effects of unitarity) which we may compare with the results of Ref. 5. Our results are much lower than those reported in Ref. 5, but this comparison may not be significant because we have neglected inelastic scattering for states in which the angular momentum $l \geq 1$.[6]

Questions of convergence are located in an Appendix which includes an example of the rate of the convergence of the Padé approximants for potential scattering which is useful in a study of Tani's work.

Faddeev[7] and Lovelace[8] have pointed out that the kernel in the n-d integral equations is singular so that the Fredholm method cannot be applied. This singularity occurs in these matrix elements: two of the three particles scatter; the momentum of the third relative to their center of mass does not change. The matrix element contains a delta function expressing this fact. Our form for the matrix element contains such a delta function. The Padé method is applicable to integral equations with singular kernels. Consider the following integral equation:

$$f(x)=h(x)+\lambda\int_{-\infty}^{\infty} dx'\delta(x-x')g(x,x')f(x').$$

The solution,

$$f(x)=h(x)/[1-\lambda g(x,x)]$$

cannot be obtained from the Fredholm method; however, the Padé approximants to the series obtained by iterating the integral equation are the solution.

[5] R. M. Frank and J. L. Gammel, Phys. Rev. **93**, 643 (1954).

[6] For experimental data, see D. E. Groce and R. E. Shamu, in *Proceedings of the International Conference on Nuclear Physics, Paris, 1964* (Editions du Centre National de la Recherche Scientifique, Paris, 1965), p. 167.

[7] For an account of Faddeev's work, see J. Gillespie, in *Final State Interactions*, (Holden-Day, Inc., San Francisco, California, 1964). For Amado's work see R. Aaron, R. D. Amado, and Y. Y. Yam, Phys. Rev. **136**, B650 (1964) and Phys. Rev. Letters **13**, 574, 701 (1964).

[8] C. Lovelace, in *Strong Interactions and High Energy Physics*, edited by R. G. Moorehouse (Plenum Press, Inc., New York 1963).

II. CONNECTION OF THE PADÉ APPROXIMANT METHOD WITH UNITARITY OF THE S MATRIX

Let the power-series expansion of the S matrix be

$$S=1+S_1V+S_2V^2+\cdots, \tag{1}$$

where the expansion parameter V is the strength of the interaction. The complex conjugate of S transposed is

$$S^\dagger=1+S_1^\dagger V+S_2^\dagger V^2+\cdots. \tag{2}$$

Unitarity requires that

$$S\cdot S^\dagger=1+(S_1+S_1^\dagger)V+(S_2+S_2^\dagger+S_1\cdot S_1^\dagger)V^2+\cdots=1, \tag{3}$$

from which it follows that

$$\begin{aligned} S_1+S_1^\dagger&=0,\\ S_2+S_2^\dagger+S_1\cdot S_1^\dagger&=0, \end{aligned} \tag{4}$$

etc.

In these equations, the center dot does not stand for multiplication in the usual sense. The S matrix for potential scattering is a function of two vectors $\mathbf{k}_f$ and $\mathbf{k}_i$, the final and initial momenta, respectively, in a scattering process. In general, unitarity requires that

$$\sum_c (a|S|c)(c|S^\dagger|b)=\delta_{ab}, \tag{5}$$

where c is summed over all states that lie on the energy shell. It follows that in the case of potential scattering, the sum over c is related to an integration over the angles of an intermediate momentum $\mathbf{k}$, since the magnitude of $\mathbf{k}$ is determined by the energy shell condition $k_f^2=k_i^2=k^2$. If we imagine that all states are normalized in a large box of volume Ω, it is easily seen that Eq. (5) is

$$\frac{1}{4\pi}\int d\hat{k}(\mathbf{k}_f|S|\mathbf{k})(\mathbf{k}|S^\dagger|\mathbf{k}_i)=\delta_{\mathbf{k}_f,\mathbf{k}_i}=\frac{(2\pi)^3}{\Omega}\delta(\mathbf{k}_f-\mathbf{k}_i), \tag{6}$$

or that the operation represented by the center dot is

$$\cdot\equiv\frac{1}{4\pi}\int d\hat{k}. \tag{7}$$

The caret notation refers to the angles of the vector $\mathbf{k}$ (i.e., $\int d\hat{k}\equiv\int d\Omega_k$). In the case of n-d scattering above the threshold for inelastic scattering, the sum over c includes an integration over the continuum states of the deuteron.

The diagonal Padé approximants are now defined in the same way they are defined in Baker's review.[1] For example, the [1,1] approximant to S is the ratio of two first-order polynomials in V:

$$S=(A_0+A_1V)\cdot\frac{1}{1+B_1V}.$$

[B_0 may be chosen to be 1, as indicated, because both

numerator and denominator may be divided by a constant.] The constants A_0, A_1, B_1 are defined by requiring that

$$(A_0+A_1V)\cdot\frac{1}{1+B_1V}=1+S_1V+S_2V^2+\cdots \tag{8}$$

to order V^2; thus

$$\begin{aligned} A_0&=1,\\ A_1&=B_1+S_1,\\ 0&=S_1\cdot B_1+S_2. \end{aligned} \tag{9}$$

The order of multiplication is important because the multiplication defined by Eq. (7) is not commutative. We have, however, the following theorem:

Theorem: The approximant defined by requiring that

$$\frac{1}{1+B_1'V}\cdot(A_0'+A_1'V)=1+S_1V+S_2V^2+\cdots$$

be satisfied to order V^2 is the same as the approximant defined by Eq. (8).

Proof: In order to prove that

$$\frac{1}{1+B_1'V}\cdot(A_0'+A_1'V)=(A_0+A_1V)\cdot\frac{1}{1+B_1V}, \tag{10}$$

multiply from the left by $1+B_1'V$ and from the right by $1+B_1V$. The result,

$$(1+A_1'V)\cdot(1+B_1V)=(1+B_1'V)\cdot(1+A_1V), \tag{11}$$

when multiplied out, contains no term of order greater than V^2. But the two approximants are equal to order V^2. Therefore, they are exactly equal.

This proof extends to diagonal $[N,N]$ Padé approximants. It is a consequence of the contraction of powers in numerator and denominator to half the largest power retained in the S matrix. The proof holds only for diagonal Padé approximants.

As a further consequence of this contraction of powers, we have the following theorem:

Theorem: The $[N,N]$ Padé approximants are exactly unitary.

Proof: The $[1,1]$ approximant is

$$[1,1]=(1+A_1V)\cdot\frac{1}{1+B_1V}, \tag{12}$$

which has a complex conjugate transposed

$$[1,1]^\dagger=\frac{1}{1+B_1^\dagger V}\cdot(1+A_1^\dagger V). \tag{13}$$

If the $[1,1]$ approximant is unitary, it is necessary that

$$[1,1]\cdot[1,1]^\dagger=(1+A_1V)\cdot\frac{1}{1+B_1V}\cdot\frac{1}{1+B_1^\dagger V}\cdot(1+A_1^\dagger V)=1. \tag{14}$$

Lemma: A necessary and sufficient condition that $AB=1$ is that $BA=1$. From Eq. (14) it follows that it is necessary and sufficient that

$$(1+A_1^\dagger V)\cdot(1+A_1V)\cdot\frac{1}{1+B_1V}\cdot\frac{1}{1+B_1^\dagger V}=1. \tag{15}$$

Multiplying from the right first by $1+B_1^\dagger V$ and then by $1+BV$ it follows that it is necessary and sufficient that

$$(1+A_1^\dagger V)\cdot(1+A_1V)=(1+B_1^\dagger V)\cdot(1+B_1V). \tag{16}$$

Again, Eq. (16) can be multiplied out and no terms of order greater than V^2 appear. But the approximant agrees with the S matrix which is unitary through order V^2, so that the approximant is exactly unitary. The argument extends to the $[N,N]$ approximant.

The argument, while correct, may at first sight seem unbelievable. An alternative proof, at least for the $[1,1]$ approximant, may be based on the solutions of Eqs. (9)

$$\begin{aligned} B_1&=-\frac{1}{S_1}\cdot S_2,\\ A_1&=S_1-\frac{1}{S_1}\cdot S_2, \end{aligned} \tag{17}$$

from which it follows that

$$\begin{aligned} B_1^\dagger&=-S_2^\dagger\cdot\frac{1}{S_1^\dagger},\\ A_1^\dagger&=S_1^\dagger-S_2^\dagger\cdot\frac{1}{S_1^\dagger}. \end{aligned} \tag{18}$$

Equations (17) and (18) may be substituted into Eq. (16), and the correctness of the result verified using Eqs. (4).

In proving these general theorems, it is correct to manipulate with the multiplication sign as we have done; however, Eqs. (9) are actually integral equations

$$\begin{aligned} (\mathbf{k}_f|A_1|\mathbf{k}_i)&=(\mathbf{k}_f|B_1|\mathbf{k}_i)+(\mathbf{k}_f|S_1|\mathbf{k}_i),\\ 0&=\frac{1}{4\pi}\int d\hat{k}(\mathbf{k}_f|S_1|\mathbf{k})(\mathbf{k}|B_1|\mathbf{k}_i)+(\mathbf{k}_f|S_2|\mathbf{k}_i), \end{aligned} \tag{19}$$

so that Eqs. (18) represent solutions of these integral equations.

Even the calculation of the Padé approximant Eq. (8) requires the solution of an integral equation. It is more convenient to work with the scattering amplitude M rather than S in order to eliminate delta functions. Let

$$S=1+2ikM, \tag{20}$$

so that Eq. (12) becomes

$$M=\frac{1}{2ik}(A_1-B_1)V\cdot\frac{1}{1+B_1V}. \tag{21}$$

Multiplying from the right by $1+B_1V$, and using the first of Eqs. (9) to eliminate A_1-B_1, application of Eq. (7) gives an integral equation for M:

$$(\mathbf{k}_f|M|\mathbf{k}_i)=\frac{1}{2ik}(\mathbf{k}_f|S_1|\mathbf{k}_i)V - \frac{V}{4\pi}\int d\hat{k}(\mathbf{k}_f|M|\mathbf{k})(\mathbf{k}|B_1|\mathbf{k}_i). \tag{22}$$

In general, this method always results in systems of integral equations which must be solved. The integrals have finite ranges (2π in azimuth, π in polar angle). There are no singularities in the integral equations. In the case of n-d scattering which we treat in Sec. IV, integrals over an energy region of allowed inelastic events will occur.

III. PARTIAL-WAVE EXPANSION OF THE SCATTERING AMPLITUDE

A partial-wave expansion of the second of Eqs. (19) gives

$$0=S_{1l}B_{1l}+S_{2l}. \tag{23}$$

From the first of Eqs. (4) it follows that S_{1l} is purely imaginary, and the imaginary part of Eq. (23) gives

$$0=\mathrm{Im}S_{1l}\,\mathrm{Re}B_{1l}+\mathrm{Im}S_{2l}. \tag{24}$$

The real part of Eq. (23) gives

$$0=-\mathrm{Im}S_{1l}\,\mathrm{Im}B_{1l}+\mathrm{Re}S_{2l}. \tag{25}$$

A partial-wave expansion of the second of Eqs. (4) gives

$$S_{2l}+S_{2l}^*+S_{1l}S_{1l}^*=0, \tag{26}$$

or, since S_{1l} is purely imaginary,

$$2\,\mathrm{Re}S_{2l}=-(\mathrm{Im}S_{1l})^2, \tag{27}$$

and this result substituted into Eq. (25) gives

$$\mathrm{Im}B_{1l}=-\tfrac{1}{2}\,\mathrm{Im}S_{1l}. \tag{28}$$

A partial-wave expansion of Eq. (22) gives

$$M_l=(1/2ik)S_{1l}V-M_lB_{1l}V. \tag{29}$$

Constructing the real and imaginary parts of B_{1l} from Eqs. (24) and (28), and putting $S_{1l}=i\,\mathrm{Im}S_{1l}$ gives

$$M_l=(1/2k)\,\mathrm{Im}S_{1l}V+M_l((\mathrm{Im}S_{2l}/\mathrm{Im}S_{1l}) +\tfrac{1}{2}i\,\mathrm{Im}S_{1l})V, \tag{30}$$

which can be solved for M_l. The tangent of the lth phase shift is given by

$$x_l=kM_l/(1+ikM_l). \tag{31}$$

Substituting the result for M_l obtained from Eq. (30) into Eq. (31) gives

$$x_l=\frac{\mathrm{Im}S_{1l}V/2}{1-V(\mathrm{Im}S_{2l}/\mathrm{Im}S_{1l})}. \tag{32}$$

The point of this argument is that Eq. (32) is exactly what would have been found by forming a Padé approximant to the power series of x_l directly. We show this fact as follows. Equation (31) expanded gives

$$x_l=kM_l-ik^2M_l^2+\cdots. \tag{33}$$

Equation (20) then gives

$$x_l=\frac{k(S_l-1)}{2ik}-ik^2\frac{(S_l-1)^2}{2ik}+\cdots, \tag{34}$$

so that Eq. (1) gives

$$x_l=(1/2i)(S_{1l}V+S_{2l}V^2)+\tfrac{1}{4}iS_{1l}^2V^2+\cdots, \tag{35}$$

or finally, using Eq. (27) for $\mathrm{Re}S_{2l}$

$$x_l=\tfrac{1}{2}\,\mathrm{Im}S_{1l}V+\tfrac{1}{2}\,\mathrm{Im}S_{2l}V^2+\cdots. \tag{36}$$

Equation (32) is obviously the ordinary [1,1] approximant to this series.

Thus we have established the following theorem:

Theorem: The solution of Eqs. (19) and (22) for M has a partial-wave expansion. The tangents of the phase shifts which appear in this partial-wave expansion are the [1,1] Padé approximants to the Born series for the tangents of the phase shifts which appear in the partial-wave expansion of the exact M.

To complete the argument, we need a proof of this theorem which holds for all $[N,N]$ Padé approximants, not just the [1,1] approximant. Again, it is the contraction of powers characteristic of the diagonal Padé approximants which assures the truth of the theorem for all N. If, in Eq. (31),

$$M_l=\frac{A_1V+\cdots+A_NV^N}{1+B_1V+\cdots+B_NV^N}, \tag{37}$$

then

$$x_l=\frac{k(A_1V+\cdots+A_NV^N)}{1+B_1V+\cdots+B_NV^N+ik(A_1V+\cdots+A_NV^N)}, \tag{38}$$

which is of the form of an $[N,N]$ approximant to x. That it must be the usual Padé approximant follows from the fact that M_l as given by Eq. (37) is correct to order V^{2N}, and therefore x_l as given by Eq. (38) is also correct to order V^{2N}, and from the fact that the Padé approximant is unique. Unitarity guarantees that x_l is real and that all of the coefficients of various powers of V in numerator and denominator of Eq. (38) are real, but it is not necessary to trace this fact in detail as we have done for the [1,1] approximant.

For a proof of the convergence of the Padé method

and examples of its rate of convergence see the Appendix.

IV. *n-d* SCATTERING

It is not obvious that an expansion such as that shown in Eq. (3) exists for *n-d* scattering. A first Born approximation exists and is given by Goldberger and Watson.[9] In the following we do not need an explicit definition of the second Born approximation; it is calculated assuming

(a) that an expansion such as that shown in Eq. (3) exists and that the first term is the first Born approximation,

(b) that this expansion has the properties shown in Eq. (4),

(c) that in the limit in which inelastic scattering is ignored, the results of Christian and Gammel[4] are obtained from the [1,1] Padé approximant, and

(d) that any parts of S_2 not required by assumptions (b) and (c) are zero.

V need not be the strength of any potential. It need not be defined at all for our purposes. We assume (a)–(d) and proceed as follows:

Let the continuum states of the deuteron be labeled by the Greek letter kappa, where

$$\kappa^2=ME/\hbar^2, \tag{39}$$

M=mass of nucleon, E=excitation energy of the deuteron. Let $k_i^2=8ME_{\rm LAB}/9\hbar^2$ be the square of the center-of-mass wave number of the incident neutron whose energy is $E_{\rm LAB}$ in the laboratory. Let

$$\alpha^2=ME_b/\hbar^2, \tag{40}$$

where E_b is the binding energy of the deuteron. Then the sum over c in Eq. (5) is such that corresponding to Eq. (7)

$$\cdot=\frac{1}{4\pi}\int d\hat{k}+\frac{1}{4\pi}\frac{\Omega}{(2\pi)^3}\int d\hat{k}\int d\boldsymbol{\kappa}, \tag{41}$$

where in the second integral the magnitude of $\mathbf{k}$ satisfies the energy-shell condition

$$-\tfrac{4}{3}\kappa^2-\tfrac{4}{3}\alpha^2+k_i^2=k^2. \tag{42}$$

The first integral allows for a transition to an intermediate state in which the deuteron is bound. The second integral allows for transitions to energetically possible intermediate states in which three particles are free. The integration over $\boldsymbol{\kappa}$ is over all vectors whose length is less than $\frac{3}{4}k^2-\alpha^2$. Below threshold, $\frac{3}{4}k^2-\alpha^2<0$, no transitions to states with three particles free are energetically possible, the second integral drops out, and the definition of multiplication reduces to that shown in Eq. (7).

[9] M. L. Goldberger and K. M. Watson, *Collision Theory* (John Wiley & Sons, Inc., New York, 1964), p. 156, Eq. (178), the first terms.

We introduce the following notation:

Let

$$(\mathbf{k}'\alpha|M|\mathbf{k}\alpha) \tag{43}$$

denote matrix elements of M between states in which the deuteron is bound. Let

$$(\mathbf{k}'\boldsymbol{\kappa}'|M|\mathbf{k}\alpha)\quad\text{and}\quad(\mathbf{k}\alpha|M|\mathbf{k}'\boldsymbol{\kappa}') \tag{44}$$

denote matrix elements of M between a state in which the deuteron is bound and a state in which three particles are free. Let

$$(\mathbf{k}'\boldsymbol{\kappa}'|M|\mathbf{k}\boldsymbol{\kappa}) \tag{45}$$

denote matrix elements of M between states in which three particles are free. At all times the k's and κ's satisfy Eq. (42).

The analogs of Eqs. (19) and (22) are

$$\begin{aligned}0=&\frac{1}{4\pi}\int d\hat{k}''(\mathbf{k}'\boldsymbol{\kappa}'|S_1|\mathbf{k}''\alpha)(\mathbf{k}''\alpha|B_1|\mathbf{k}\boldsymbol{\kappa})\\&+\frac{1}{4\pi}\frac{\Omega}{(2\pi)^3}\int_0^{\frac{3}{4}k^2-\alpha^2}d\boldsymbol{\kappa}''\\&\times\int d\hat{k}''(\mathbf{k}'\boldsymbol{\kappa}'|S_1|\mathbf{k}''\boldsymbol{\kappa}'')\\&\times(\mathbf{k}''\boldsymbol{\kappa}''|B_1|\mathbf{k}\boldsymbol{\kappa})+(\mathbf{k}'\boldsymbol{\kappa}'|S_2|\mathbf{k}\boldsymbol{\kappa}),\end{aligned} \tag{46}$$

$$\begin{aligned}(\mathbf{k}'\boldsymbol{\kappa}'|M|\mathbf{k}\boldsymbol{\kappa})=&\frac{1}{2ik}(\mathbf{k}'\boldsymbol{\kappa}'|S_1|\mathbf{k}\boldsymbol{\kappa})\\&-\frac{V}{4\pi}\int d\hat{k}''(\mathbf{k}'\boldsymbol{\kappa}'|M|\mathbf{k}''\alpha)(\mathbf{k}''\alpha|B_1|\mathbf{k}\boldsymbol{\kappa})\\&-\frac{V}{4\pi}\frac{\Omega}{(2\pi)^3}\int d\boldsymbol{\kappa}''\\&\times\int d\hat{k}''(\mathbf{k}'\boldsymbol{\kappa}'|M|\mathbf{k}''\boldsymbol{\kappa}'')\\&\times(\mathbf{k}''\boldsymbol{\kappa}''|B_1|\mathbf{k}\boldsymbol{\kappa}).\end{aligned} \tag{47}$$

In these equations, $\boldsymbol{\kappa}'$ may be α and $\boldsymbol{\kappa}$ may be α also. Equations (46) and (47) express the fact that unitarity is bound to connect the processes [nucleon+ground state of deuteron → nucleon+ground state of deuteron], [nucleon+ground state of deuteron → nucleon +continuum state of deuteron], and [nucleon+continuum state of deuteron → nucleon+continuum state of deuteron]. It would be nice if it were possible to avoid the third possibility, and so eliminate all matrix elements such as $(\mathbf{k}'\boldsymbol{\kappa}'|M|\mathbf{k}\boldsymbol{\kappa})$ where neither $\boldsymbol{\kappa}'$ nor $\boldsymbol{\kappa}$ is α, but it is not possible.

The solution of Eqs. (46) and (47) is not difficult if the dependence of all matrix elements on the angles of the $\boldsymbol{\kappa}$'s can be eliminated. In general this dependence

cannot be eliminated, but in the present work our approximations used in calculating S_1 and S_2 achieve this for matrix elements not of the form $(\mathbf{k}'\boldsymbol{\kappa}'|S|\mathbf{k}\boldsymbol{\kappa})$ where neither $\boldsymbol{\kappa}'$ nor $\boldsymbol{\kappa}$ is α. However, we need this form of the matrix element for S_1. We will write down a reasonable-looking form which is independent of the direction of $\boldsymbol{\kappa}'$ and $\boldsymbol{\kappa}''$.

When the angles of the $\boldsymbol{\kappa}$'s do not appear, a partial-wave expansion of Eqs. (46) and (47) is easily carried out precisely as a partial-wave expansion was carried out in Sec. III. Equations (46) and (47) become one-dimensional integral equations which we have solved only for the orbital angular momentum $l=0$. For $l\geq 1$, we have used the phase shifts of Christian and Gammel.[4] It would be easy to include other l's, and this may be necessary to explain the low inelastic cross sections we calculate.

V. FURTHER DETAILS OF THE CALCULATION

The spin complicates the problem somewhat. But for central forces the total spin is a good quantum number, so that the doublet and quartet states may be dealt with separately. For the doublet state, both deuteron singlet and triplet states are accessible, so that larger matrices occur: In a schematic way we have the following form for any $S=\frac{1}{2}$ matrix:

	ground state	triplet continuum	singlet continuum
	α	κ	κ
α	(1)	(3)	(2)
κ		(4)	(5)
κ			(6)

In (1) are the matrix elements between states in which the deuteron is bound. (2) contains matrix elements

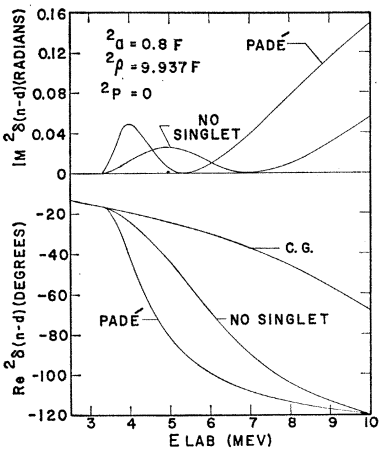

FIG. 1. Energy dependence of doublet phase shifts. C. G. stands for Christian and Gammel (Ref. 4). For the "no singlet" curve the singlet continuum states of the deuteron were neglected.

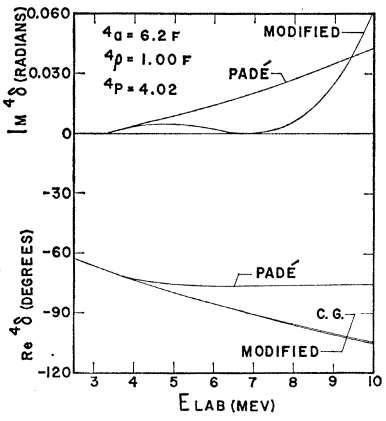

FIG. 2. Energy dependence of quartet phase shifts. "Modified" means that all parts of S_2 were computed using Eq. (54).

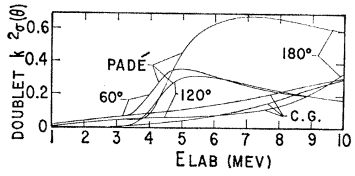

FIG. 3. Doublet contribution to $k^2\sigma$ for several angles.

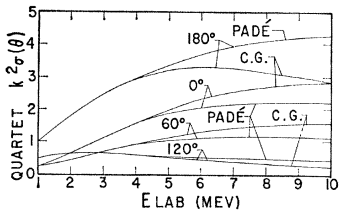

FIG. 4. Quartet contribution to $k^2\sigma$ for several angles.

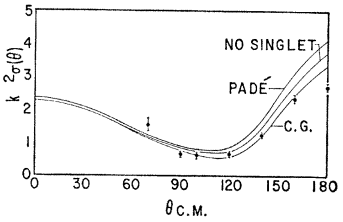

FIG. 5. Angular distribution at $E_{\text{LAB}}=5$ MeV.

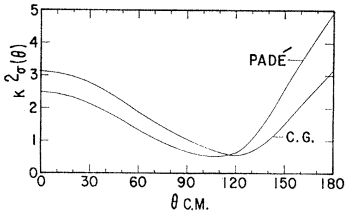

FIG. 6. Angular distribution at $E_{\text{LAB}}=10$ MeV.

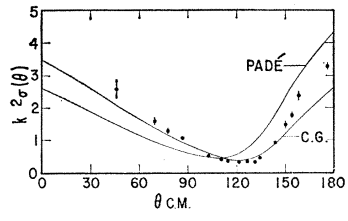

FIG. 7. Angular distribution at $E_{\text{LAB}}=14$ MeV.

between a state in which the deuteron is bound and a state in which all particles are free, two being in a singlet continuum state of the deuteron.

The spin factors in front of matrix elements have been worked out in Refs. 4 and 5. The calculation of the matrix elements in zero range approximation is also explained in Refs. 4 and 5. We find, for $l=0$,

$$(k\alpha|S_1|k\alpha)=-i\beta\frac{8\alpha}{3k}\ln\left(\frac{(9/4)k^2+\alpha^2}{\frac{1}{4}k^2+\alpha^2}\right), \quad (48)$$

$$\mathrm{Re}(k'\kappa'|S_1|k\alpha)=\beta\frac{1-\cos 2\delta_0(\kappa')}{2\kappa'}\left\{\frac{16\sqrt{\pi}}{3k'}\left(\frac{\alpha}{2}\right)^{1/2}\times\ln\left(\frac{(\frac{1}{2}k+k')^2+\alpha^2}{(\frac{1}{2}k-k')^2+\alpha^2}\right)\right\}$$

$$=-\mathrm{Re}(k\alpha|S_1|k'\kappa'), \quad (49)$$

$$\mathrm{Im}(k'\kappa'|S_1|k\alpha)=\beta\frac{\sin 2\delta_0(\kappa')}{2\kappa'}\{\quad\}$$

$$=\mathrm{Im}(k_0\alpha|S_1|k'\kappa'), \quad (50)$$

where β is the spin factor ($\beta=+1$ for quartet states, $-\frac{1}{2}$ for doublet states except for transitions to states in which the deuteron is in a singlet continuum state, in which case $\beta=(\sqrt{\frac{3}{2}})\times 0.69$, when 0.69 is the ratio of the strengths of the singlet and triplet n-p potentials), and where $\delta_0(\kappa')$ is a triplet or singlet n-p phase shift depending on whether the matrix element goes in (3) or (2) in the schematic drawing for $S=\frac{1}{2}$; for $S=\frac{3}{2}$, the singlet continuum states do not occur.

In practice, the integral in Eq. (41) which remains after partial-wave expansion is approximated by a finite sum. After partial-wave expansion, Eq. (41) becomes

$$\cdot=1+\frac{1}{(2\pi)^3}\times 4\pi\int\kappa^2 d\kappa, \quad (51)$$

(the Ω is absorbed in the matrix elements above). The factors $F(\kappa)=(1/2\pi^2)\kappa^2\Delta\kappa$ are also absorbed in the

TABLE I. Inelastic cross section $\sigma_{\mathrm{in}}=(\pi/k^2)[1-\exp(-4\,\mathrm{Im}\delta)]$.

E_{LAB} (MeV)	${}^4\sigma_{\mathrm{in}}$ (F^2)	${}^2\sigma_{\mathrm{in}}$ (F^2)	σ_{in} (mb)
4	0.514	6.411	21
6	1.333	0.828	11
8	1.879	4.782	28
10	2.308	6.554	38
14	2.800	6.900	41

TABLE II. Effect of variation of parameters on fit to inelastic e-d cross section: $E_{\mathrm{LAB}}=5.5$ MeV.

			$k^2\sigma(\theta)$ and σ_{in}							
	Reδ (deg)	Imδ (rad)	$\theta=0°$	30°	60°	90°	120°	150°	180°	σ_{in} (mb)
Quartet contribution										
Result of varying the part of S_2 given by Eq. (55)										
S_2 [Eq. (55)]										
−1.01	−65	0.036	1.59	1.36	0.82	0.41	0.55	2.22	3.89	36
−2.02	−76	0.011	1.98	1.71	1.09	0.55	0.53	1.98	3.53	12
−3.03	−88	0.000	2.30	2.01	1.31	0.65	0.45	1.63	3.02	0
Result of varying the ${}^4P$ phase shift										
${}^4P$ phase shift										
0.37			1.43	1.27	0.89	0.55	0.55	1.77	3.12	12
0.47			1.98	1.71	1.09	0.55	0.53	1.98	3.53	12
0.56			2.66	2.27	1.33	0.55	0.50	2.18	3.90	12
Result of varying a factor inserted on the right-hand side of Eq. (52)										
Factor										
5	−80	0.000	2.12	1.85	1.19	0.60	0.51	1.87	3.36	6
1	−76	0.011	1.98	1.71	1.09	0.55	0.53	1.98	3.53	12
$\frac{1}{5}$	−70	0.036	1.76	1.52	0.94	0.46	0.53	2.11	3.71	36
Doublet contribution										
Result of varying the part of S_2 given by Eq. (55)										
S_2 [Eq. (55)]										
1.3	63	0.054	0.26	0.24	0.22	0.21	0.24	0.45	0.66	52
2.6	88	0.000	0.37	0.36	0.35	0.33	0.32	0.43	0.57	0
3.9	−76	0.015	0.36	0.36	0.35	0.33	0.28	0.31	0.40	16
Result of varying a factor inserted on the right-hand side of Eq. (52)										
Factor										
5	−48	0.29	0.22	0.33	0.24	0.22	0.15	0.09	0.13	29
1	88	0	0.37	0.36	0.35	0.33	0.32	0.43	0.57	0
$\frac{1}{5}$	68	0.46	0.28	0.27	0.25	0.23	0.27	0.46	0.65	45

TABLE III. Effect of variation of parameters on fit to inelastic e-d cross sections: $E_{LAB}=14$ MeV.

	Reδ (deg)	Imδ (rad)	$k^2\sigma(\theta)$ and σ_{in} $\theta=0°$	30°	60°	90°	120°	150°	180°	σ_{in} (mb)
Quartet contribution										
Result of varying the part of S_2 given by Eq. (55)										
S_2										
−1.59	−69	0.15	1.98	1.45	0.84	0.37	0.38	2.07	3.96	48
−3.18	−75	0.076	2.21	1.65	1.00	0.48	0.43	2.04	3.90	28
−4.79	−79	0.038	2.40	1.81	1.11	0.55	0.44	1.97	3.78	15
Result of varying a factor inserted on he right-hand side of Eq. (52)										
Factor										
4	−81	0.015	2.49	1.89	1.17	0.58	0.45	1.95	3.74	6
1	−75	0.076	2.21	1.65	1.00	0.48	0.43	2.04	3.90	28
$\frac{1}{5}$	−81	0.16	2.16	1.47	0.73	0.42	1.16	1.92	3.75	54
Result of varying the ^4P phase shift										
^4P phase shift										
0.38			1.59	1.20	0.80	0.48	0.45	1.80	3.43	28
0.48			2.21	1.65	1.00	0.48	0.43	2.04	3.90	28
0.57			2.97	2.21	1.24	0.48	0.40	2.26	4.32	28
Doublet contribution										
Result of varying the part of S_2 given by Eq. (55)										
S_2										
0	42	0.42	0.23	0.17	0.08	0.07	0.08	0.20	0.36	85
0.77	53	0.27	0.27	0.23	0.12	0.10	0.11	0.26	0.44	69
1.53	61	0.17	0.35	0.29	0.17	0.15	0.16	0.32	0.50	52
Result of varying a factor inserted on the right-hand side of Eq. (52)										
Factor										
5	54	0.108	0.36	0.30	0.16	0.13	0.15	0.33	0.52	37
1	53	0.27	0.27	0.23	0.12	0.10	0.11	0.26	0.44	69
$\frac{1}{5}$	51	0.35	0.27	0.21	0.11	0.09	0.10	0.24	0.40	79
Result of varying the ^2P phase shift										
^2P phase shift										
−0.5 rad			0.68	0.57	0.33	0.10	0.22	1.00	1.62	69
0			0.27	0.23	0.12	0.10	0.11	0.26	0.44	69
0.5 rad			1.88	1.42	0.53	0.10	0.09	0.07	0.036	69

matrix elements [every term in (2) and (3) in the schematic drawing for $S=\frac{1}{2}$ would get a factor $\sqrt{F(\kappa)}$], and multiplication is now ordinary matrix multiplication. At the end points, an additional factor $1/\sqrt{2}$ is absorbed in the matrix elements.

In (4), (5), and (6) of the schematic drawing, we put zeros everywhere except on the diagonal (thus (5) has all zeros); on the diagonal we put

$$(k\kappa|S_1|k\kappa)=-i\tfrac{2}{3}k_0(\sin 2\delta_0(\kappa)/\kappa), \tag{52}$$

which includes the factor $F(\kappa)$. These elements of S_1 are proportional to a delta function $\delta(\kappa-\kappa')$, which is replaced by $1/\Delta\kappa$ on the diagonal in a finite mesh, which is canceled by the $\Delta\kappa$ in $F(\kappa)$.

The second Born approximation was calculated from unitarity. We assumed, in accord with assumption (d), that except for one element of S_2,

$$S_2-S_2^{\dagger}=0, \tag{53}$$

so that

$$S_2=\tfrac{1}{2}S_1\cdot S_1. \tag{54}$$

For the part of S_2 in (1) we did not put the imaginary part of S_2 equal to zero but put in a number such that if inelastic scattering is neglected altogether the Padé approximant we form gives the scattering matrix of Christian and Gammel[4] [this is assumption (c)]. We took, therefore,

$$\mathrm{Im}(k\alpha|S_2|k\alpha)=\mathrm{Im}(k\alpha|S_1|k\alpha)\times\left[1-\frac{\mathrm{Im}(k\alpha|S_1|k\alpha)}{2\tan\delta_0(n-d)}\right], \tag{55}$$

where $\delta_0(n$-$d)$ are the doublet or quartet S n-d phase shifts of Ref. 4. We have from Eq. (32), in the limit in which inelastic scattering is ignored,

$$x_0=\mathrm{Im}S_1/2[1-(1-\mathrm{Im}S_1/2\tan\delta_0)]=\tan\delta_0$$

as it should, thus verifying the form of Eq. (55).

VI. RESULTS

1. The Energy Dependence of the Phase Shifts

Above threshold, the phase shifts become complex. In Figs. 1 and 2 the energy dependence of the phase

shifts is exhibited. Christian and Gammel's phase shifts, which must be used in Eq. (55), were calculated from fits to their effective-range plots. Effective-range parameters which fit their plots are given on Figs. 1 and 2. In the doublet case, the curve marked "no singlet" was calculated omitting the deuteron singlet continuum states. In the quartet case, the curves marked "modified" were calculated using Eq. (54) for all parts of S_2 [thus omitting the part given by Eq. (55)].

The doublet and quartet contributions to $k^2\sigma(q)$ (including statistical weight factors) are shown in Figs. 3 and 4 for several angles as a function of E_{LAB}.

Several angular distributions for elastic n-d scattering are shown in Figs. 5, 6, and 7. In a qualitative way, the results of Christian and Gammel are not violently affected.

The total inelastic cross section is given in Table I as a function of energy. Christian and Gammel adjusted their S phase shifts to fit the data, and also their ^4P phase shift. We also have varied certain parameters to see what effect this has on the fits to the data. The results are tabulated in Tables II and III. The parameters varied were the ^4P phase shift, the part of S_2 given by Eq. (55), and the diagonal part of S_1 given by Eq. (52). While we have not given an adequate derivation of Eq. (52), wide variations in a numerical factor inserted on the right-hand side do not affect the elastic angular distributions, as the tables show.

VII. CONCLUSIONS

We have mainly demonstrated the feasibility of these calculations. Much more care should be put into the next stage of work. The zero-range approximation is not at all essential. As a matter of principle, we need to know how to compute Eq. (52) correctly. We should not use Eq. (54), and should compute the second Born approximation $S_2-S_2^\dagger$ for all parts of the S matrix, not just the part given by Eq. (55). We should compute the part of S_2 given by Eq. (55) from first principles to justify Eq. (55). Like Lovelace [see p. 472, line 31, sentence beginning with "Thirdly," of Ref. 8], we are somewhat uncertain that our S matrix is related to what experimentalists measure. These improvements are feasible.

Inclusion of tensor and spin-orbit terms in the two-nucleon interaction is a question of extremely tedious detail. Hard cores can be handled in the Padé scheme but the [1,1] approximant may not be sufficient to include them accurately. To compute the [2,2] approximant seems impossible at present. These improvements may not be feasible.

Our results for the real and imaginary parts of the phase shifts above threshold for inelastic scattering will be useful for comparing with similar results obtained from the new attack on this problem initiated by Amado, Faddeev, and Lovelace.[7,8]

APPENDIX

It is known that the sequence of Padé approximants to the Born series for tangents of phase shifts converges for Yukawa potentials (see Refs. 1 and 3) because these series are series of Stieltjes. The sequence of Padé approximants which we have defined do not depend on a partial-wave expansion, and their convergence depends on the uniformity (with respect to l) of convergence of the series for the tangents of the phase shifts, because infinitely many l's are involved. The validity of the first Born approximation increases in such a way that, given ϵ, there exists L such that

$$|\sum_{l=L}^{\infty}(S_lP_l-S_{l\,\text{Born}}P_l)|<\epsilon/2. \tag{A1}$$

Then given ϵ and this L there exists an order of Padé approximation N, such that for all $l<L$

$$|S_lP_l-[N,N]_lP_l|<\epsilon/2L.$$

Assuming that the $[N,N]_l$ approach S_l in such a way that $[N,N]_l$ is closer to S_l than $S_{l\,\text{Born}}$ (which follows from the fact that the Padé approximants to series of Stieltjes converge from one side), Eq. (A1) gives

$$|\sum_{L}^{\infty}S_lP_l-[N,N]_lP_l|<\epsilon/2, \tag{A2}$$

which combined with Eq. (40) gives

$$|\sum S_lP_l-[N,N]_lP_l|<\epsilon. \tag{A3}$$

Thus for potential scattering the use of unitarity and solution of the resulting integral equations such as Eqs. (19) and (22) is not different from forming Padé approximants to the Born series for the tangents of the phase shifts. In more complicated cases, such as n-d scattering, with inelastic scattering present, when the phase-shift method is not available, it offers something new.

Of course the *rate* of convergence is of importance. This rate is easily established for simple examples, for example the scattering length of a square-well potential.[10] The Schrödinger equation for this example is

$$-(\hbar^2/2M)(d^2\psi/dx^2)+V(x)\psi=0,$$

where $V(x)=+V$ for $x<c$ and $V(x)=0$ for $x>c$. For $x<0$

$$\psi=\sinh[(2MV/\hbar^2)^{1/2}x],$$

and for $x>0$

$$\psi=x+a.$$

Joining these two solutions at $x=c$ gives

$$\frac{a}{c}=-1+\frac{\tanh[(2MV/\hbar^2)^{1/2}c]}{(2MV/\hbar^2)^{1/2}c}.$$

[10] G. A. Baker and J. L. Gammel, J. Math. Anal. Appl. 2, 21, 405 (1961).

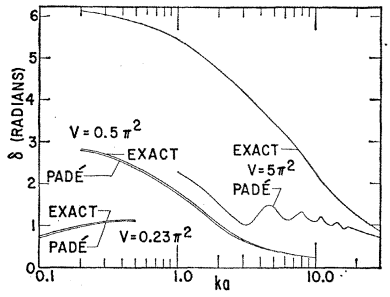

FIG. 8. S phase shift as a function of κa for several potential strengths.

Letting $w=2MVc^2/\hbar^2$, the Born series for a/c is

$$\frac{a}{c}=-\frac{1}{3}w^2+\frac{2}{15}w^4+\cdots.$$

The [1,1] approximant to this is

$$\frac{a}{c}=-\frac{\frac{1}{3}w^2}{(1+\frac{2}{5}w^2)}.$$

For $w^2\to\infty$; that is, for $V\to\infty$, $a/c\to-5/6$ as compared with the exact answer $a/c=-1$. The [2,2] approximant gives $a/c=-14/15$, the [3,3] $a/c=-24/25$. The spectacular rate of convergence of the method is known in several problems.[1]

The pole in the denominator for a/c is in the correct place: The [1,1] approximant begins to fail if the potential is attractive and strong enough to bind two states: In that case the [2,2] approximant is necessary. However, for n-d scattering, the triton has only one bound state, and the [1,1] approximant should be adequate. For pion-nucleon scattering, there are no bound states.

For energies $E>0$, by matching boundary conditions as in the example for $E=0$,

$$\frac{\tan\delta}{k}=\frac{(2MV/\hbar^2k^3)B(k)}{1-(2MV/\hbar^2k^2)D(k)},$$
$$B(k)=\tfrac{1}{2}(ka-\sin ka\cos ka),\tag{A4}$$
$$D(k)=\frac{1}{4B(k)}[ka\sin^2ka+\tfrac{1}{2}\sin ka\cos ka-\tfrac{1}{2}ka-ka\cos^2ka+\sin ka\cos^3ka].$$

TABLE V. Phase shifts for infinite repulsive potential given by the exact expression and the [1,1] approximant.

ka	[1,1]	$-[1,1]/ka$
0	−0.00	0.833
0.5	−0.41	0.828
1.0	−0.82	0.820
1.5	−1.21	0.806
2.0	−1.56	0.780
3.1416	−2.05	0.670

This result obviously approaches the Born approximation (which appears in the numerator) as the energy ($k^2=2ME/\hbar^2$) approaches infinity. The [1,1] approximant is valid at all energies as long as there is no more than one bound state. It begins to break down as the potential becomes strong enough to give one bound state *and* a resonance, or two bound states. In those problems in which several bound states occur, say $N>1$ so that the phase shift is $N\pi$ at zero energy, the [1,1] approximation becomes valid only at very high energies. One might suppose that it becomes valid as soon as the phase shift decreases to π, but such is not the case. In Fig. 8, we compare the phase shifts computed from the exact formula

$$\tan\delta=\frac{k\cos ka-\kappa\cot\kappa a\sin ka}{\kappa\cot\kappa a\cos ka+k\sin ka},$$

where

$$\kappa=\left(\frac{2MV}{\hbar^2}+k^2\right)^{1/2},$$

and the [1,1] approximant Eq. (A4) for several potentials of different strengths.

For repulsive potentials, the [1,1] approximant will not give a phase shift which passes through $(-\pi)$. It will give a phase shift which passes through $(-\pi/2)$, and this case is relevant to quartet n-d scattering, especially Eq. (55).

For an infinitely repulsive potential, the exact expression $\delta=-ka$ and the [1,1] approximant are compared in Table V.