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Richard Webb Haymaker

July 13, 1967

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THE APPLICATION OF ANALYTICITY PROPERTIES TO THE NUMERICAL SOLUTION OF THE SCHRÖDINGER AND BETHE-SALPETER EQUATIONS

Richard Webb Haymaker
July 13, 1967
(Ph. D. Thesis)
ERRATA

TO: All recipients of UCRL-17652
FROM: Technical Information Division

Please correct subject report as follows:

Page 34: Eq. (4.25f) should read \( q = -i \sigma \mu /2 \), \( \sigma \geq 1 \).

Page 45: In Eq. (6.12), the \( Y_{n}^{l} m(\hat{r}) \) on the right-hand side should be \( Y_{l}^{m}(\hat{r}) \).

Page 47: In Eq. (6.17), the functions \( Y_{n}^{l} \ell^0(\hat{x}) \) and \( \phi_{j}(R) \) should be \( Y_{n}^{l} \ell^0(\hat{x}) \) and \( \phi_{j}^{*}(R) \), respectively.

Page 47: Eq. (6.18) should read

\[
V_{lj} = (2\pi)^{2} \int d^{4}x \frac{J_{n+1}(|k|R)}{|k|R} V(x) \phi_{j}^{*}(R).
\]

Page 80: Eq. (C.15) should read

\[
i(2j+1) \ M_{ij} = (2i-1)(j+1) M_{i-1,j+1} - (2j+1)(i-1) M_{i-2,j+1} + (2i-1)j M_{i-1,j-1}.
\]
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THE APPLICATION OF ANALYTICITY PROPERTIES TO THE NUMERICAL SOLUTION OF THE SCHröDINGER AND BETHE-SALPETER EQUATIONS

Richard Webb Haymaker

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July 13, 1967

ABSTRACT

A new method of calculating phase shifts from the Bethe-Salpeter equation is presented. The differential equation is solved below threshold using a variational method and then the scattering amplitude is continued to the physical scattering region using Padé approximants. The singularity structure of the Schrödinger and Bethe-Salpeter amplitudes in their off-shell variables was studied to find the nearby singularities that could most strongly affect the continuation. A variational method of calculating Regge trajectories in potential theory is presented. The variational equations are derived in the bound state region and then continued directly to all values of angular momentum and energy.
I. INTRODUCTION

Throughout the development of a theory of strong interactions, the problem of doing reliable dynamical calculations has remained a difficult one. The calculation of two body scattering amplitudes for example entails the inclusion of a variety of many particle effects, the sequence of importance of which is still poorly defined. Our quantitative understanding of strong interactions rests heavily on model calculations which try to ascertain the importance of the ingredients that are known to be present from first principles, i. e. unitarity, crossing, covariance, inelastic channels, etc.

The approaches to strong interaction dynamics can be mainly classified as on-mass-shell methods that arise from the analytic S-matrix\(^1,2\) approach and field theoretic methods which yield off-mass-shell equations.\(^3\) Our concern will be with the latter but our point of view will be that the off-shell equations are a starting point for doing dynamics, much like the role of the Schrödinger equation in non-relativistic quantum mechanics.

Historically, on-shell methods have played a major role for dealing with the two body problem. However now that methods have been developed to solve realistic two body relativistic off-shell equations\(^4-6\) (Bethe-Salpeter equations\(^7-9\)), we feel that this will be a more fruitful approach for numerical calculations in the future for a number of reasons. The non-relativistic problem can be phrased in both languages and it turns out to be far simpler to integrate the Schrödinger equation
than to solve the N/D equations\textsuperscript{10} with the same physical content. The reason is that only a potential function is needed as input to the off-shell equation whereas the discontinuity across the whole left hand cut of the scattering amplitude must be given as input to the N/D equations. There are of course an infinite number of contributions to the left hand cut, one coming from each term in the Born series. It is particularly important to keep many terms for repulsive potentials since the contributions from successive terms alternate in sign. Another on-shell method is the Mandelstam iteration scheme\textsuperscript{11} which enables one to calculate the double spectral function, but this is also quite difficult to carry out in practice.\textsuperscript{12} The non-relativistic three body problem has been handled traditionally by off-shell equations (the Faddeev equations\textsuperscript{13}) where only recently have three body N/D equations been proposed.\textsuperscript{14} Progress has been made in solving relativistic off-shell three body equations\textsuperscript{15} whereas no attempt to solve the corresponding on-shell equations is known to the author.

The objection to the Bethe-Salpeter equation is that an off-mass-shell continuation of the scattering amplitude is necessarily used. Since the scattering amplitude can be measured only for the mass-shell values of external momenta the continuation off the mass-shell is arbitrary. A natural analytic continuation off the mass-shell is not among the fundamental axioms of S-matrix theory.

There has been a revival of interest in off-shell equations for physical models partly because of the shortcomings of the practical solutions of the N/D equations. The pion-nucleon system has been re-
investigated using the Bethe-Salpeter equation. Blankenbecler and Sugar have developed a three dimensional approximation to the Bethe-Salpeter equation and used it to re-examine the Zachariasen-Zemach bootstrap of the rho meson. Also the method of effective potentials is a scheme to phrase the ideas of S-matrix theory in a Schrödinger theory language for the purpose of doing calculations, and has seen numerous applications.

We will be concerned mainly with the Bethe-Salpeter equation in the ladder approximation. It is similar in form to the Schrödinger equation but is four dimensional and relativistically covariant. It embodies crossing but produces an amplitude satisfying elastic unitarity only in the direct channel. The Bethe-Salpeter amplitude has an infinite number of inelastic thresholds corresponding to production processes. It also has the four dimensional symmetry for total energy equal to zero which gives rise to the daughter sequence of Regge trajectories. Like the Schrödinger equation only a potential or interaction kernel is needed as input.

In this thesis the analytic structure of the solutions of the Schrödinger and Bethe-Salpeter equations is studied and applied to methods of calculation. A knowledge of the singularities is necessary for most methods of solving the equations, e.g. for the removal of singularities in the integral equations, or the development of quadrature formulae. We use the knowledge of the analytic structure to perform numerical continuations to find phase shifts from the scattering amplitude in the bound state region. The amplitude can
be calculated easily from the differential equation in this region and the problems of solving a singular integral equation for the phase shifts are avoided.\textsuperscript{6,22,23} The analytic continuation to the scattering region is carried out using \textsuperscript{28} approximants.

Section II consists of preliminary remarks introducing the off-mass-shell Bethe-Salpeter equation and appropriate variables. In Secs. III to V we find all the singularities of the Schrödinger scattering amplitude in its off-shell variables, and a large class of singularities of the Bethe-Salpeter amplitude.\textsuperscript{29} It is our main concern to find the singularities near the elastic threshold that can most strongly affect the numerical continuation. In Secs. VI and VII the details of calculating the scattering amplitude below threshold and continuing it to the scattering region are given. Both off-mass-shell and on-mass-shell continuations are presented and compared. Finally in Sec. VIII a Rayleigh-Ritz variational method of finding Regge trajectories in potential theory is presented in which the variational equations are derived in the bound state region and then continued directly to all complex values of angular momentum and energy.\textsuperscript{30,31}
II. OFF-SHELL CONTINUATION

We consider the two particle Bethe-Salpeter equation with a local potential as a starting point following Schwartz and Zemach. 5

\[ \psi_{k_1 k_2}(x_1, x_2) = \psi_{k_1 k_2}^0(x_1, x_2) \]

\[ + \int \frac{d^4 x_1}{\hbar} \frac{d^4 x_2}{\hbar} G_{k_1 k_2}(x_1, x_2; x_1', x_2') I(x_1', x_2') \psi_{k_1 k_2}(x_1', x_2'), \]

where \( x_1 = (x_1, t_1) \). The free wave term \( \psi^0 \) is \( \exp[i(k_1 \cdot x_1 + k_2 \cdot x_2)] \), \( G \) is the free two particle Green's function and \( I(x_1, x_2) \) is the interaction kernel. The \( T \) matrix for the scattering process \( k_1 + k_2 \rightarrow k'_1 + k'_2 \) is:

\[ T(k'_1, k'_2; k_1, k_2) = i \int \frac{d^4 x_1}{\hbar} \frac{d^4 x_2}{\hbar} \psi_{k'_1 k'_2}^{0*}(x_1, x_2) I(x_1, x_2) \psi_{k_1 k_2}(x_1, x_2). \]

(2.2)

Using translational invariance it is possible to reduce this equation to a four dimensional equation. Consider the new coordinates and momenta:

\[ X = v_1 x_1 + v_2 x_2 \]

\[ x = x_1 - x_2 \]

\[ K = k_1 + k_2 = k'_1 + k'_2 \]

\[ k = v_2 k_1 - v_1 k_2 \]

\[ k' = v_2 k'_1 - v_1 k'_2. \]

(2.3)
The fact that \( I(x_1, x_2) \) depends only on \( x \) is the statement of translational invariance which implies:

\[
\psi_{k_1, k_2}(x_1, x_2) = e^{iK \cdot X} \psi_{k, k}(x). \tag{2.4}
\]

Substituting this into Eq. (2.1) gives

\[
\psi_{k, K}(x) = \psi_k^0(x) + \int \frac{dx'}{4} G_K(x - x') I(x') \psi_{k, K}(x'). \tag{2.5}
\]

where:

\[
\psi_k^0(x) = e^{i k \cdot x}, \tag{2.6}
\]

\[
G_K(x - x') = \int \frac{dp}{(2\pi)^4} e^{i p \cdot (x - x')} \tilde{G}_K(p), \tag{2.7}
\]

\[
\tilde{G}_K(p) = \frac{1}{[(v_1 K + p)^2 + m_1^2 - i\epsilon] [(v_2 K - p)^2 + m_2^2 - i\epsilon]} \tag{2.8}
\]

We have used the condition \( v_1 + v_2 = 1 \), which assures that \( d^4 x_1 d^4 x_2 = d^4 X d^4 x \) and \( k_1 \cdot x_1 + k_2 \cdot x_2 = K \cdot X + k \cdot x \). A small negative imaginary part is attached to all internal masses to define the integrals which gives causal boundary conditions on the scattered wave. Finally the \( T \) matrix becomes:

\[
T(k', k, K) = i \int d^4 x \psi_{k, K}^*(x) I(x) \psi_{k, K}(x), \tag{2.9}
\]
Thus we have defined the scattering amplitude as a function of three independent vectors $k$, $k'$, and $K$, the functional dependence on each is clearly shown in Eqs. (2.5) and (2.9), and we have thereby defined an off-mass-shell continuation of the $T$ matrix. We note in particular that the free wave term depends only on $k$, and the Green's function depends only on $K$. Clearly there are in fact six invariants that can be formed from these three vectors and can be related to the usual variables $s$, $t$, and the four external masses $k_1^2$, $k_2^2$, $k_1'^2$, $k_2'^2$ through Eqs. (2.3).

It should be mentioned that the Bethe-Salpeter equation as presented above is not yet amendable to a partial wave analysis. This is because $G_K(x - x')$ is not a rotationally invariant function of $(x - x')$. There are terms of the form $(x - x') \cdot K$ since $G_K(p)$ contains the term $K \cdot p$. This can be remedied of course by going to the center of mass frame where $K = (E, 0)$. The Schrödinger equation however can be made rotationally invariant in the relative coordinate in an arbitrary Galilean frame. For this case the Green's function is

$$g_E(x - x') = \int \frac{d^3p}{(2\pi)^3} e^{i\mathbf{p} \cdot (x - x')} \tilde{g}_K(p), \quad (2.10)$$

$$\tilde{g}_K^{-1}(p) = \left(\frac{v_1 K + p}{2m_1}\right)^2 + \left(\frac{v_2 K - p}{2m_2}\right)^2 - E - i\epsilon. \quad (2.11)$$

By choosing $v_1 = m_1/(m_1 + m_2)$, the $K \cdot p$ term drops out and

$$\tilde{g}_K^{-1}(p) = \frac{p^2}{2\mu} + \frac{K^2}{2M} - E - i\epsilon, \quad (2.12)$$
where \( \mu = m_1 m_2 / (m_1 + m_2) \), and \( M = (m_1 + m_2) \). This complete separation of the center of mass motion is not possible for the Bethe-Salpeter equation. This reflects the fact that a rotationally invariant system does not remain rotationally invariant in an arbitrary Lorentz frame.

Going to the center of mass system, and further setting \( E = 0 \) so that the full vector \( K \) is zero, it is clear that \( G_K(x - x') \) is an invariant function of \( (x - x') \) under all Lorentz transformations. Since the vector \( K \) enters only in the Green's function this produces a symmetry of the wave function and the \( T \) matrix under all Lorentz transformations that act on the relative vectors leaving the total momentum vector \( K \) alone. This implies the daughter sequence of Regge trajectories\(^{21,32}\) and was apparent in earlier bound state calculations.\(^4,9\)

In the center of mass system, the \( T \) matrix is normalized such that

\[
T_{k',k} = \frac{8\pi E}{k} \sum_l (2l + 1) P_l(\cos \theta) e^{i\theta \sin \delta} , \quad (2.13)
\]

where \( T_{k,k} \) is the on-mass-shell value of \( T(k', k, K) \), i.e. \( K = (E, 0) \), and \( k^2 = k^2 = -m^2 \).

For a one particle exchange force of mass \( \mu \),

\[
I(x) = -16 i \pi^2 \lambda \int d^4p \frac{e^{i p \cdot x}}{p^2 + \epsilon} ,
\]

\[
= \frac{\hbar \mu}{|x|} K_1(\mu|x|) , \quad (2.14)
\]
where $K_1$ is the modified Bessel function. Going to momentum space, the integral equation for the $T$ matrix is

$$T(k', k, K) = \tilde{V}(k' - k) - i \int \frac{d^4 p}{(2\pi)^4} \tilde{V}(k' - p) \tilde{G}_K(p) T(p, k, K), \quad (2.15)$$

where

$$\tilde{V}(k' - k) = i \int d^4 x e^{-i(k' - k) \cdot x} \tilde{I}(x) = \frac{16 \lambda x^2}{(k - k')^2 + \mu^2 - i\epsilon}. \quad (2.16)$$

Equations (2.5) and (2.15) are inhomogeneous equations for the scattering problem. The corresponding homogeneous equations are eigenvalue equations for the bound state energies. This can be seen most easily from Eq. (2.14) since a bound state manifests itself as a pole in the $T$ matrix.

Equation (2.15) can be represented diagrammatically as in Fig. 1 as the sum of the Born series or ladder series. The diagrams are to be interpreted literally as Feynman diagrams. It is the four dimensional character of the equation that produces inelastic thresholds. Roughly, the emission and absorption of particles on the rungs of the ladder need not occur at the same time and thus if the energy is high enough, production of these ladder rung particles is possible. A similar diagrammatic interpretation can be given to the Schrödinger equation where the diagrams represent terms in non-relativistic perturbation theory. The Schrödinger equation is of course three dimensional, not involving the relative time, and the rungs of the ladder are emitted and absorbed at
the same time thus not allowing for production. In Sec. IV we show in detail how inelastic thresholds are generated.

We will also need the Schrödinger equation, and it is given here for future reference. The $T$ matrix equation is

$$T(k', k, E) = V(k' - k) + \int d^3p \frac{1}{2} \sum_{\tilde{W}} \frac{1}{\tilde{p}^2 - E - i\epsilon} T(p, k, E).$$

(2.17)

Referring to Eq. (2.12) it is clear that we have set the reduced mass $\mu$ equal to $\frac{1}{2}$ and absorbed the energy of the center of mass into $E$.

$$V(k' - k) = \frac{-\lambda}{2\pi^2} \frac{1}{(k' - k)^2 + \mu^2},$$

(2.18)

$$T(q', q, E) = \frac{1}{2\pi^2} \sum_{\ell} (2\ell + 1) p_{\ell}(\hat{q}, \hat{q}') e^{i\ell} \sin \theta_{\ell}$$

(2.19)

where in the last equation $|q| = |q'| = (E)^{\frac{1}{2}}$. 

III. SINGULARITIES OF THE OFF-SHELL SCHröDINGER PARTIAL WAVE AMPLITUDE

Our interest is primarily in the partial wave amplitude since this is the function one computes in practice. Let us define the amplitude as follows:

\[ T^\ell(k', k, q) = \frac{kk'}{2} \int_{-1}^{+1} d\cos\theta \, P^\ell(\cos\theta) T(k', k, E), \quad (3.1) \]

where \( k, k' \), etc., \( q^2 = E \). The on-shell singularities in the variable \( E = k^2 = k'^2 \) are well known, i.e. the left hand cut depending on the range of the potential, the right hand cut starting at threshold and the bound state poles if the potential strength is large enough. For our purposes we would like to know the singularity structure of \( T^\ell \) in its three variables separately. There are singular hypersurfaces in the six dimensional \( k', k, q \) complex space for which the on-shell constraints pick out one two dimensional complex plane.

The partial wave amplitude \( T^\ell(k', k, q) \) satisfies the following integral equation:

\[ T^\ell(k', k, q) = \bar{\chi} B^\ell(k', k) + \bar{\chi} \int_0^\infty dp \, B^\ell(k', p) B^\ell(k, q) T(p, k, q), \quad (3.2) \]

where

\[ B^\ell(k', k) = -Q^\ell \left( \frac{k^2 + k'^2 + \mu^2}{2kk'} \right), \quad B^\ell(k, q) = \frac{k\pi}{p^2 - q^2 - i\epsilon}, \quad (3.3) \]
and \( \tilde{\lambda} = \sqrt{\frac{\hbar}{\pi m^2}} \) was defined for convenience. For sufficiently small \( \tilde{\lambda} \), this equation can be solved by iteration giving the Born series:

\[
T_{\ell}(k', k, q) = \sum_{n=1}^{\infty} (\tilde{\lambda})^n B_{\ell}^{(n)}(k', k, q), \quad (3.4)
\]

where

\[
B_{\ell}^{(n)}(k', k, q) = \int_{0}^{\infty} dp B_{\ell}(1)(k', p) G(p) B_{\ell}^{(n-1)}(p, k, q). \quad (3.5)
\]

The amplitude \( T_{\ell} \) will have the singularities of all the Born terms. The singularity structure of the first Born term is trivial. But since the \( n \)th Born term is defined as an integral over the first term and the \( (n - 1) \)th term, standard mathematical methods of finding singularity positions of functions defined by integrals may be used to find the singularity positions of all the Born terms without doing the integrals explicitly or examining multiple integrals.

If the potential is sufficiently attractive there will also be poles corresponding to bound states. These poles are not in the Born series and thus if bound states are present, the Born series must diverge.\(^{33}\) The bound states are solutions to the homogeneous equation corresponding to Eq. (3.2) and it is clear that their position in \( q \) will be independent of \( k \) and \( k' \).

Our task in this section is to find the singularities of the Born series. These are branch points whose positions are simple functions
of the momenta and range of the potential. The bound state pole positions can only be found by numerical solution of the equation.

For simplicity let \( l = 0 \). The results we find will hold for any physical \( l \) because the singularities of \( B^{(1)}(k', k) \) and the kernel of the integral equation are independent of \( l \). Dropping the \( l \) subscript,

\[
B^{(1)}(k', k) = \log \left( \frac{(k' + k)^2 + \mu^2}{(k' - k)^2 + \mu^2} \right). \tag{3.6}
\]

Consider \( B^{(2)}(k', k, q) \):

\[
B^{(2)}(k', k, q) = \int_0^\infty dp \log \left( \frac{(k' + p)^2 + \mu^2}{(k' - p)^2 + \mu^2} \right) \frac{4\pi}{p^2 - q^2 - i\epsilon} \log \left( \frac{(p+k)^2 + \mu^2}{(p-k)^2 + \mu^2} \right). \tag{3.7}
\]

The lower limit of the integration can be extended to \(-\infty\) because the integral is an even function of \( p \).

The singularity structure of the integrand in Eq. (3.7) in the \( p \) plane is shown in Fig. 2a. The cuts come from the logarithms and the poles from the Green's function. The contour \( \Gamma \) is along the real axis. Singularities of the integral can occur only when singularities of the integrand approach the contour from opposite sides and pinch against each other in such a way that the contour can not be deformed to avoid the pinch. The conditions for pinches to occur are the following:
The column to the right of Eqs. (3.8) refers to the type of pinch, i.e. $G$ means Green's function pole, $B(1)$ and $B(1)'$ refer to the right and left logarithmic branch points in Eq. (3.7). There are additional pinches if $\mu$ is variable, but we shall not consider them.

We notice the following points concerning these singularities:

(a) For $q$ in the upper half plane, the poles at $p = \pm q$ can not pinch the contour against other singularities in the $p$ plane showing that the upper half $q$ plane is analytic. The left hand cut is absent in this variable.

(b) Equation (3.8d) can be disposed of as not producing a singularity. This is because the integrand can be written as the sum of two terms, one containing the branch points at $p = \pm k + i\mu$ and the other containing

<table>
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<th>$q = 0$</th>
<th>$G$</th>
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<tr>
<td>$q = \pm k - i\mu$</td>
<td>$G B(1)$</td>
<td>(3.8b)</td>
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<tr>
<td>$q = \pm k' - i\mu$</td>
<td>$B(1)' G$</td>
<td>(3.8c)</td>
</tr>
<tr>
<td>$k = \pm i\mu$</td>
<td>$B(1) B(1)$</td>
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<td>$k' = \pm i\mu$</td>
<td>$B(1)' B(1)'$</td>
<td>(3.8e)</td>
</tr>
<tr>
<td>$k = \pm k' \pm 2i\mu$</td>
<td>$B(1)' B(1)$</td>
<td>(3.8f)</td>
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</tbody>
</table>
the branch points at \( p = \pm k - i\mu \). Obviously when the integrand can be written as the sum of these two terms, the singularities can not pinch. The same considerations hold for Eq. (3.8a).

(c) We can determine the type of singularity produced by the "GG pinch," Eq. (3.8a), by passing the contour \( \Gamma \) above the pole at \( p = q \) in Fig. 2a to the contour \( \Gamma_1 \) picking up the residue of the pole. In this way the integral is separated into two parts, one which does not have a pinch as \( q \) goes to zero and the residue which is known explicitly:

\[
B^{(2)}(k',k,q) = \int_{\Gamma_1} + \frac{k^2 q^2}{q} \log \left( \frac{(k' + q)^2 + \mu^2}{(k' - q)^2 + \mu^2} \right) \log \left( \frac{(k + q)^2 + \mu^2}{(k' - q)^2 + \mu^2} \right).
\]

(3.9)

The integrand in formula (3.7) depends on \( q^2 \) only. The pinch between the two "G poles" produces a branch point in \( q^2 \) at \( q^2 = 0 \). This can be seen in Eq. (3.9) since the integral along \( \Gamma_1 \) has no singularity at \( q^2 = 0 \), the residue contribution however is seen to be proportional to \( q \) for small \( q \).

(d) The "GB\(^{(1)}\)" and "GB\(^{(1)}\)'" pinches are between a pole and a logarithmic branch point. The resulting branch point in the integral is logarithmic as can be seen by distorting the contour \( \Gamma \) to \( \Gamma_2 \) shown in Fig. 2a, picking up the residues of the poles at \( p = \pm q \). For \( q \) now in the lower half plane, the integral along \( \Gamma_2 \) is free of singularities. The residues of the two poles are equal and are given in Eq. (3.9). We notice that this term has singularities in the upper half \( q \) plane also, but they must be cancelled by the integral along \( \Gamma_2 \) since the original integral along \( \Gamma \) does not have them.
(e) The "B(1) B(1)'" pinch, Eq. (3.8f), is between two logarithmic branch points. The resulting singularity is not a simple logarithm. Isolating one particular pinch, e.g. \( k + i\mu = -k' - i\mu \), we can use the results of Appendix A to find the discontinuity around the branch point caused by this pinch. The discontinuity in the \( k \) plane going once around the branch point at \( k = -k' - 2i\mu \) is

\[
\Delta B^{(2)}(k', k, q) = -4i\pi \int_{k' - i\mu}^{k + i\mu} dp \frac{1}{p^2 - q^2}.
\]

(3.10)

Close to the branch point, \( \Delta B^{(2)}(k', k, q) \sim (k + k' + 2i\mu) \).

The singularities of the second Born term are summarized in Fig. 2b,c.

In like manner the singularities of the third Born term can be found from Eq. (3.5):

\[
B^{(3)}(k', k, q) = \frac{1}{g^2} \int_{-\infty}^{\infty} dp B^{(1)}(k', p) g_q(p) B^{(2)}(p, k, q).
\]

(3.11)

Referring to Fig. 3a, the equations for pinches are the following:

\[
\begin{align*}
q^2 &= 0 & \text{GG} & \quad (3.12a) \\
q &= \pm k' - i\mu & B^{(1)} & \quad (3.12b) \\
q &= \pm k - 2i\mu, q = -i\mu/2 & G B^{(2)} & \quad (3.12c) \\
q + i\mu &= \pm k - i\mu & B^{(1)} & \quad (3.12d) \\
\pm k' - i\mu &= \pm k + 2i\mu & B^{(1)} B^{(2)} & \quad (3.12e)
\end{align*}
\]
\[
\begin{align*}
q + i\mu &= \pm k - 2i\mu \quad \text{(3.12f)} \\
q &= -i\mu \quad \text{(3.12g)} \\
k &= \pm 2i\mu \quad \text{(3.12h)}
\end{align*}
\]

We have omitted those conditions that are known by the above arguments to produce no singularity.

The new features that occur for this case are the following:

(a) There are no singularities at the positions given by Eq. (3.12f, h). This is because \(B^{(n)}(k', k, q)\) is symmetric in \(k\) and \(k'\) and there is no mechanism to produce the singularity at the corresponding value of \(k'\).

(b) Also there is no singularity at \(q = -i\mu\) [Eq. (3.12g)] because the singularities that pinch appear as a sum. (See discussion of the second Born term.)

(c) There are singularities of \(B^{(2)}(p, k, q)\) that do not depend on the integration variable \(p\), and thus must be included as they are. In particular \(B^{(2)}(p, k, q)\) has singularities at \(q = \pm k - i\mu\), which are necessary in order for \(B^{(3)}(k', k, q)\) to be symmetric in \(k\) and \(k'\). [See Eq. (3.12b)].

(d) The discontinuities can be calculated using the results of Appendix A though this has not been done.

It is easy to see that these arguments generalize to \(B^{(n)}(k', k, q)\). It has the following singularity positions:
\[ q^2 = 0 \]

\[ q = -j \frac{i \mu}{2} \]

\[ k = \pm k' \pm n i \mu \]  \hspace{1cm} (3.13)

\[ q = \pm k' - n i \mu \]

\[ q = \pm k - n i \mu \]

where \( m = 1, 2, \ldots, (n - 1) \), \( j = 1, 2, \ldots, (n - 2) \). On the energy shell \( (q = k = k' = \frac{1}{\hbar} E^2) \) the above equations reduce to

\[ E = 0 \]

\[ \frac{1}{E} = \pm \frac{n i \mu}{2} \]  \hspace{1cm} (3.14)

\[ \frac{E}{\hbar} = -\frac{n i \mu}{2} \]

\[ \frac{1}{E} = \infty. \]

The singularities of all the Born terms are present in the full partial wave amplitude.
IV. SINGULARITIES OF THE OFF-MASS-SHELL BETHE-SALPETER PARTIAL WAVE AMPLITUDE

A. Partial Wave Ladder Series.

The analysis of the singularities of the off-mass-shell Bethe-Salpeter partial wave amplitude is considerably more complicated than for the non-relativistic problem of the previous section. This amplitude is a function of more variables and there is an integration over the time component in the equations. This amplitude is defined in the usual way:

\[ T_{\ell}(k',k',\omega) = \frac{kk'}{8\pi^2} \int_{-1}^{+1} d\cos \theta P_{\ell}(\cos \theta) T(\kappa,\kappa,\omega) \]  

where \( \kappa = (k',k') \) and \( \kappa' = (k',k') \). (Throughout this section \( k \) and \( k' \) will refer to the magnitudes of the three vectors \( \kappa \) and \( \kappa' \).) For convenience we introduce \( \omega = E/2 \) and \( q = \sqrt{\omega^2 - m^2} \).

With this definition,

\[ T_{\ell}(q,0,q,0,\omega) = -\left(\frac{2}{\pi}\right)^2 q \omega e^{i\delta_{\ell}} \sin \delta_{\ell}. \]

We have restricted ourselves to equal mass scattering of particles with mass \( m \), interacting through a single particle exchange of mass \( \mu \).

Our primary interest is to find the singularity structure of \( T_{\ell} \) in the variable \( q \) close to elastic threshold. There are two different continuations that are of interest for the numerical work that follows which govern the emphasis of this section. The first is a continuation in \( q \) from the bound state region to the scattering region.
holding \( k \) equal to \( k' \) and at the point where the phase shift is desired. The second is again a continuation in \( q \) but with \( k \) and \( k' \) constrained to the mass-shell, i.e. \( q = k = k' \). For both cases \( k_0 = k'_0 = 0 \). In practice we will have to find the singularities for a much larger domain of these variables since they are found by iterating the equation as was done in the previous section.

A great deal has been studied about the Feynman diagrams (not partial wave analysed) that appear in the ladder series (Fig. 1) that is generated by the Bethe-Salpeter equation. We will study the partial wave analysed graphs and make comparisons where possible with the full Feynman graphs for complementary information on the singularity structure.

The partial wave Bethe-Salpeter equation for the \( T \) matrix is

\[
T_\ell(k', k'_0, k, k_0; \omega) = \left( \frac{2\lambda}{\pi} \right) B_\ell^{(1)}(k', k'_0, k, k_0)
+ \left( \frac{2\lambda}{\pi} \right) \int_0^\infty dp \int_{-\infty}^\infty dp_0 B_\ell^{(1)}(k', k'_0, p, p_0)
\times G_{\omega}(p, p_0) T_\ell(p, p_0, k, k_0; \omega),
\]

where

\[
B_\ell^{(1)}(k, k'_0, k, k_0) = -Q_\ell \left( \frac{k^2 + k'^2 - (k - k'_0)^2 + \mu^2}{2kk'} \right),
\]

and
The Born or ladder series is

\[ T_{\beta}(k',k,k',\omega) = \sum_{n=1}^{\infty} \left( \frac{2\lambda}{\pi} \right)^n B_{\beta}^{(n)}(k',k',k,k',\omega), \quad (4.6) \]

where

\[ B_{\beta}^{(n)}(k',k',k,k',\omega) = \int_0^\infty dp \int_{-\infty}^\infty dp_0 B_{\beta}^{(1)}(k',k',p,p_0) G_{\omega}(p,p_0) \]

\[ \times B_{\beta}^{(n-1)}(p,p_0,k,k',\omega). \quad (4.7) \]

In Part B below, we discuss some of the known simple properties of Feynman diagrams that are relevant to our discussion. In Part C we find all the singularities of \( B_{\beta}^{(2)} \) in all variables by direct examination of Eq. (4.7). Part D is devoted to a discussion of how these singularities propagate themselves in the ladder series.

B. Feynman Diagrams.

Certain singularities that occur in the Feynman diagrams of the ladder series may be taken over directly to our problem. The partial wave diagrams are defined as integrals of Feynman diagrams over \( \cos \Theta \), and those singularities whose positions are independent of \( \cos \Theta \) will remain. There is a large class of such singularities that we will review from the extensive literature. \[ 34 \]
Consider the box diagram in Fig. 4a, whose partial wave counterpart is the second Born term in Eq. (4.7). This has the following singularities that are independent of \( \cos \theta \):

(i) There are normal thresholds

\[
4 \omega^2 = -(k_1 + k_2)^2 = (m \pm m)^2. \quad (4.8)
\]

The solution with the minus sign lies on the second sheet of the branch point at \( \omega^2 = m^2 \) and is thus "far away" from the bound state region.35 This relation between two solutions occurs very often below and usually only one solution will be of interest.

(ii) There are also normal thresholds for each of the external particles separately, for example

\[
k_1^2 = -(m \pm \mu)^2, \quad (4.9)
\]

where again the \( (m - \mu) \) solution is on the second sheet of the \( (m + \mu) \) solution.

(iii) The triangle singularity which is obtained by contracting36 one of the \( \mu \) particle internal lines, shown in Fig. 4b, is another example. Its position is given by the following equation:37

\[
Y_1^2 + Y_2^2 + Y_3^2 + 2 Y_1 Y_2 Y_3 - 1 = 0, \quad (4.10)
\]

where:
This is a "moving singularity" in that its position depends on more than one external invariant. The sheet structure of this surface with respect to the normal thresholds is discussed very clearly in the literature, and we shall not review it here though it is important for Part C below.

These results are summarized in Fig. 4. The box diagram has the singularities of all the graphs that occur by contracting internal lines, a sample of which are presented.

Consider now an "N-rung" ladder graph, Fig. 5a. The singularities of all lower order graphs that have at least one rung contracted will be independent of \( \cos \theta \) and therefore will be present in the partial wave amplitude. Fig. 5b illustrates one such diagram that contains the \( M \)th inelastic threshold, \( (M < N - 2) \).

\[
4\omega^2 = (2m + M\mu)^2 . \tag{4.11}
\]

For this discussion the four external masses were considered independent variables \( k_1^2, k_2^2, k_1'^2, k_2'^2 \). It is convenient to transform
to the variables that appear in the Bethe-Salpeter equation for comparison with the results below. These variables are

\[ k_0^2 = \frac{(k_1^2 - k_2^2)^2}{(16\omega^2)}, \]

\[ k_0'^2 = \frac{(k_1'^2 - k_2'^2)^2}{(16\omega^2)}, \]

\[ k^2 = \omega^2 + \frac{1}{2} (k_1^2 + k_2^2) + \frac{(k_1^2 - k_1'^2)^2}{(16\omega^2)}, \]

\[ k'^2 = \omega^2 + \frac{1}{2} (k_1'^2 + k_2'^2) + \frac{(k_1^2 - k_1'^2)^2}{(16\omega^2)}. \]

C. Singularities of \( B^{(2)} \).

As for the non-relativistic problem, we consider \( \ell = 0 \) for the sake of clarity with no loss of generality. The second Born term is:

\[ B^{(2)}(k', k_0', k, k_0) = \frac{1}{2} \int_{-\infty}^{\infty} dp \int_{-\infty}^{\infty} dp_0 \log \left( \frac{S_3}{S_4} \right) \frac{1}{S_5 S_6} \log \left( \frac{S_1}{S_2} \right). \]

The integrand is singular on the surfaces \( S_1 = 0 \), where:

\[ S_1 = (k - p)^2 - (k_0 - p_0)^2 + \mu^2 \]

\[ S_2 = (k + p)^2 - (k_0 - p_0)^2 + \mu^2 \]

\[ S_3 = (k' - p)^2 - (k'_0 - p'_0)^2 + \mu^2 \]

(Equation continued)
-25-

\[ S_4 = (k' + p)^2 - (k'_0 - p_0)^2 + \mu^2 \]

\[ S_5 = p^2 - (p_0 - \omega)^2 + m^2 \]

\[ S_6 = p^2 - (p_0 + \omega)^2 + m^2 \]  \hspace{1cm} (4.14)

These surfaces can trap the hypercontour and cause singularities in the external variables. Since the integral is two dimensional, one, two, or three of these surfaces can participate in trapping the hypercontour. It is clear that Formula (4.13) can be written as the sum of four terms each containing \( S_1 \) or \( S_2 \), \( S_3 \) or \( S_4 \). And thus the interaction of \( S_1 \) and \( S_2 \), \( S_3 \) and \( S_4 \) can produce no singularities. In that which follows we will consider only the integral containing \( S_1 \), \( S_3 \), \( S_5 \) and \( S_6 \), and it should be kept in mind that there are singularities due to three other integrals that can be found by appropriate replacements of \( k \rightarrow -k \), and \( k' \rightarrow -k' \) in the final results.

The conditions for a hyper-pinch to occur in which \( m \) surfaces participate are:

\[ m = 1 \quad S_1 = 0, \quad \frac{\partial S_1}{\partial p} = 0, \quad \frac{\partial S_1}{\partial p_0} = 0 ; \]  \hspace{1cm} (4.15a)

\[ m = 2 \quad S_1 = 0, \quad S_j = 0, \quad \frac{\partial S_1}{\partial p} = \frac{\partial S_j}{\partial p} = \frac{\partial S_j}{\partial p_0}, \quad i \neq j ; \]  \hspace{1cm} (4.15b)

\[ m = 3 \quad S_1 = 0, \quad S_j = 0, \quad S_k = 0, \quad i \neq j \neq k \neq 1. \]  \hspace{1cm} (4.15c)
The surfaces $S_1 = 0$ are hyperbolas in the real $p, p_0$ plane as shown in Fig. 6a. The Feynman prescription of giving all internal masses a small negative imaginary part is used to remove all singularities from the integration path and thus define the integrals. If we hold $p$ fixed and real and look in the $p_0$ complex plane, the upper and lower branches of the hyperbolas in Fig. 6a lie in the lower and upper half complex $p_0$ plane in Fig. 6b respectively. Since the contour must be trapped at each stage of integration to produce a singularity in the integral it is clear that we need consider only those solutions in which an upper branch of a hyperbola pinches with a lower branch for only these branches pinch in the $p_0$ integration.

We will examine in turn the solutions to Eqs. (4.15a,b,c) in which one, two, and three surfaces participate.

(i) One Surface

First consider singularities generated by a single surface through Eq. (4.15a). These equations can be solved immediately and give singularities at $m^2 = 0$ and $\mu^2 = 0$. But since we are holding the masses fixed and finite, these solutions are not of interest.

(ii) Two Surfaces

Next consider the interaction of two singular surfaces in producing singularities, Eq. (4.15b). For $S_5$ and $S_6$, these equations give the elastic threshold branch point at

$$\omega^2 = m^2,$$  (4.16a)

and the well known second sheet branch point at
\[ \omega^2 = 0. \quad (4.16b) \]

The hypercontour is trapped at

\[ p = p_0 = 0. \quad (4.16c) \]

These solutions have a nice pictorial interpretation in terms of Fig. 6a. The positions of the hyperbolas \( S_5 \) and \( S_6 \) are functions of the external variable \( \omega \). When a lower branch is tangent to an upper branch we get the hyper-pincho at \( \omega^2 = m^2 \). And when a lower (upper) branch is tangent to a lower (upper) branch we get the solution \( \omega = 0 \) but the hypercontour is not pinched. However, if we start at this solution and take \( \omega \) on a path that encircles the branch point at \( \omega = m \) once and return to \( \omega = 0 \), we will find that the \( p_0 \) contour is pinched!

Because of the special importance of the normal threshold to our analytic continuation, it is shown in Appendix B, without relying on the Born series, that this pinch produces a two sheeted "square root type" branch point in the partial wave amplitude.

The surface \( S_1 \) and \( S_3 \) generate the following surfaces

\[ (k - k')^2 - (k_0 - k_0')^2 + 4\mu^2 = 0, \quad (4.17a) \]

\[ (k - k')^2 - (k_0 - k_0')^2 = 0, \quad (4.17b) \]

the hyper contour being trapped at
\[ p = \frac{k + k'}{2}, \quad p_0 = \frac{k_0 + k'_0}{2}. \]  

(4.17c)

The same considerations apply to the solution (4.17b) that were discussed above for Eq. (4.16b). Remembering that the masses have a small negative imaginary part, \(-i\epsilon\), we can see this yet in another way. The solution (4.17a) gives a singularity for real values of all the variables only when \(\epsilon \to 0\), whereas the second solution, (4.17b), exists for real values of the variables for non-zero \(\epsilon\). However, we know that the integral is non-singular for real values of these variables, the \(-i\epsilon\) being introduced solely for that purpose.

It is worthwhile examining how the surfaces \(S_1\) and \(S_3\) trap the hypercontour to produce the surface (4.17a). We will not consider the topological problem of how two surfaces trap a third one at a point, but rather will examine the integral at the alleged singular point and show that the singularities of the integrand approach the contour from opposite sides at each stage of integration.

Define

\[ \tilde{p} = p - \frac{k + k'}{2}, \]

\[ \tilde{p}_0 = p_0 - \frac{k_0 + k'_0}{2}. \]

(4.18)

Substitute these in \(S_1 = 0\) and \(S_3 = 0\), attach the \(-i\epsilon\) to the masses and choose external variables such that Eq. (4.17a) is satisfied.
These two surfaces should pinch at $\tilde{p} = \tilde{p}_0 = 0$ as $\varepsilon \to 0$.

\[ S_1 = \tilde{p}^2 + (k - k') \tilde{p} - \tilde{p}_0^2 - (k_0 - k'_0) \tilde{p}_0 - i\varepsilon = 0, \]

\[ S_2 = \tilde{p}^2 - (k - k') \tilde{p} + \tilde{p}_0^2 + (k_0 - k'_0) \tilde{p}_0 - i\varepsilon = 0. \]  

Holding $\tilde{p}$ fixed and small, the roots of these equations corresponding to small $\tilde{p}_0$ lie on opposite sides of the $\tilde{p}_0$ contour. So we can eliminate $\tilde{p}_0$ from these equations:

\[ \frac{\tilde{p}^2 - (k - k')^2}{(k_0 - k'_0)^2} \tilde{p}^2 - i\varepsilon = 0. \]  

Since the external variables are constrained by Eq. (4.17a) and if $\mu \neq 0$, then the two roots of this equation approach each other from opposite sides of the $\tilde{p}$ contour as $\varepsilon \to 0$.

The singularities due to $S_1$ and $S_4$, $S_2$ and $S_3$, and $S_2$ and $S_4$ follow immediately and are given in Table 1.

Finally the last type of two surface pinch is for example between $S_1$ and $S_5$ producing the surfaces

\[ k^2 - (k_0 - \omega)^2 + (m + \mu)^2 = 0, \]

\[ k^2 - (k_0 - \omega)^2 + (m - \mu)^2 = 0. \]
Again we can discard the second solution. All the singularities of this type are summarized in Table 1. It should be mentioned that these solutions are precisely the individual particle normal thresholds given for the full Feynman graph in Eq. (4.9) expressed in the variables (4.12).

(iii) Three Surfaces

Finally there is the case in which three surfaces participate in trapping the contour. The simplest case is the combination $S_1, S_5, S_6$, giving

$$ (k - q)^2 - k_0^2 + \mu^2 = 0 $$

$$ (k + q)^2 - k_0^2 + \mu^2 = 0 $$

where $q^2 = \omega^2 - m^2$. These solutions are just the "triangle singularity" presented in Eq. (4.10) in terms of the variables (4.12).

As was alluded to earlier, the sheet structure of this singularity in relation to the normal thresholds is not simple. But the work has been done for us to straighten out this structure\textsuperscript{38} and we need only interpret the results in terms of our variables. This has been done and is shown in Fig. 7. This surface $T_{1,5,6}$ is tangent to the lower order surfaces $T_{1,5}$ and $T_{1,6}$. If we pass along the surface $T_{1,5,6}$ from the solid portion, passing the point of tangency, the singularity goes onto the second sheet of the normal thresholds $T_{1,5}$ and $T_{1,6}'$ shown in Fig. 7b.
The last and most complicated case is the three surface pinch generated by the surfaces \( S_1, S_2 \) and \( S_5 \):

\[
\begin{align*}
\left( k'^2 - (k_0' - \omega)^2 + \mu^2 - m^2 \right) (k_0 - \omega) - \left( k^2 - (k_0 - \omega)^2 + \mu^2 - m^2 \right) (k_0' - \omega) \right)^2 \\
- \left( k'^2 - (k_0' - \omega)^2 + \mu^2 - m^2 \right) k - \left( k^2 - (k_0 - \omega)^2 + \mu^2 - m^2 \right) k' \right)^2 \\
+ 4 m^2 [k'(k_0 - \omega) - k(k_0' - \omega)]^2 = 0.
\end{align*}
\]

\( (4.23) \)

This surface and the corresponding ones shown in Table 1 are the only ones that do not reduce to conic forms in the left leg variables \( k_0', k' \). The key to picturing the surface \( T_1, 3, 5 \) is to look at its asymptotes in the \( k_0', k' \) plane. This curve is asymptotic to the lines

\[
\begin{align*}
(k_0' - \tilde{k}_0')^2 = (k' - \tilde{k}')^2, \\
\end{align*}
\]

where

\[
\tilde{k}_0' = \omega + \frac{(k_0 - \omega)}{2} \left[ 1 \mp \left( \frac{k^2 - (k_0 - \omega)^2 + (m + \mu)^2}{k^2 - (k_0 - \omega)^2} \right)^{\frac{1}{2}} \right], \quad (4.24b)
\]

and

\[
\tilde{k}' = \frac{k}{2} \left[ 1 \mp \left( \frac{k^2 - (k_0 - \omega)^2 + (m + \mu)^2}{k^2 - (k_0 - \omega)^2} \right)^{\frac{1}{2}} \right]. \quad (4.24c)
\]

The important thing to note is that for the right leg variables on the mass-shell, i.e., \( k = q, k_0 = 0 \), these asymptotes are complex.
One can also show that the surface does not intersect the real $k', k'_0$ plane under these conditions. This situation persists for $k \neq q$ for those values of $k$ and $q$ of interest for the continuations we do.

The singularities of the second Born term are displayed in yet another way in Fig. 8. These are the relevant complex planes for the two numerical continuations. For both cases we have set $k'_0 = k''_0 = 0$. Fig. 8a shows the singularities in $q$ for fixed $k = k'$, and Fig. 8b shows the analytic structure in the variable $q = k = k'$. It appears that we have left out the singularities (12) and (13) of Table 1 in the second figure. However, they are not on the exposed sheets as will be shown below in Section V on unitarity.

**D. Iteration of Singularities in the Born Series.**

With our knowledge of all the singularities of the second Born term $B^{(2)}(k', k'_0, k, k'_0, \omega)$ in the left leg variables $k', k'_0$, we could in principle find all the singularities of the third Born term using Eq. (4.7) and continue the process to find all singularities of the full partial wave amplitude as was done for the Schrödinger amplitude. To carry this out we must find the singularities for unrestricted values of $k'$ and $k'_0$ at each stage since they are integrated over in the next stage. For unrestricted values of $k, k'_0$ and $q$ the problem is quite difficult. However, if we restrict these variables to the values of interest for our numerical continuations we can find the singularities that most strongly affect the continuations. In addition we list some of the singularities of the $N$th Born term that are "far away" from the region of interest but arise in a simple way.
The majority of the singularities of $B^{(2)}$ are hyperbolic surfaces in the integration variables $p, p_0$ (See Table 1). This is a great simplification in that the complexity of the surfaces does not increase upon iteration. There are surfaces though that are not hyperbolic (Eqs. (12) and (13) of Table 1), but for $k_0 = 0$ and $k = q$, they do not intersect the real $k', k_0$ plane and thus are not potent in producing pinches in higher Born terms for the hypercontour in the real $p, p_0$ plane. As mentioned earlier this situation persists for $k \neq q$ for the regions of interest.

Restricting ourselves to just the hyperbolic surfaces we can write down a large class of singularities for $B^{(N)}_2(k', k_0, k, k_0, \omega)$ and can classify them as follows:

(i) Normal thresholds in $\omega^2$:

\[ 4 \omega^2 = (2m + \sigma \mu)^2, \quad (4.25a) \]

\[ q = -im. \quad (4.25b) \]

(ii) Normal thresholds for each leg:

\[ k^2 - (k_0 \pm \omega)^2 + (m + (\sigma + 1) \mu)^2 = 0, \quad (4.25c) \]

\[ k'^2 - (k'_0 \pm \omega)^2 + (m + (\sigma + 1) \mu)^2 = 0. \quad (4.25d) \]
(iii) Triangle type singularities:

\[(k^2 + q)^2 - k_0^2 + ((\sigma + 1) \mu)^2 = 0, \quad (4.25e)\]

\[(k'^2 + q)^2 - k_0'^2 + ((\sigma + 1) \mu)^2 = 0. \quad (4.25f)\]

(iv) Singularities on the imaginary axis:

\[q = -i(\sigma + 1) \mu/2, \quad (4.25g)\]

where \(\sigma = 0, 1, \ldots, (N - 2)\).

The iteration appears to generate many more surfaces. A large class can be ruled out using the symmetry of \(\mathcal{B}^N(k', k_0', k, k_0, \omega)\) under \(k \rightarrow k'\) and \(k_0 \rightarrow k_0'\). There are many more triangle type singularities, but just as the ones mentioned Eqs. (4.25e,f) are on the second sheet of the lowest threshold (see Fig. 9a), the other triangle type singularities are on the second sheets of higher normal thresholds. Figure 9 displays these singularities for the continuations of interest.
V. INFORMATION ON SINGULARITIES FROM ON-SHELL UNITARITY

A. Discontinuity Relation.

It is well known that the Schrödinger scattering amplitude satisfies an elastic unitarity relation, which for the partial wave amplitude allows one to define a real phase shift. The Bethe-Salpeter equation in the ladder approximation also generates a unitary amplitude although only for a finite region of energy. Generalized unitarity equations have been studied extensively, and it has been found that when combined with analyticity assumptions about the amplitude, they generate the singularities that are present in Feynman diagrams. We will show how the elastic on-shell unitarity equation gives us some information on the analyticity properties of the Bethe-Salpeter amplitude in the on-shell energy variable relevant to our continuation problem.

The unitarity equation for the partial wave S matrix, \( S_{s} = \exp(2i \Phi_{s}) \), is

\[
S_{s}(E) S_{s}^{*}(E) = 1, \tag{5.1}
\]

which simply states that the phase shift is real.

Unitarity is a non-analytic condition because of the complex conjugation, and holds only in the scattering region. However, if we assume that the amplitude is a real analytic function, real below threshold, we can write an analytic relation (called a discontinuity relation) that coincides with unitarity in the physical region:
\[ S_\ell(E_+)S_\ell(E_-) = 1, \quad (5.2) \]

where \( E_+ \) is an energy in the scattering region and \( E_- \) is that energy obtained by circling once around the elastic threshold as shown in Fig. 10a. In continuing Eq. (4.2) to general values of \( E_+ \), \( E_- \) follows \( E_+ \) but on the sheet obtained by circling threshold once. For \( E_+ \) in the scattering region, we recover unitarity because \( E_+ = E_- \) there and since \( S_\ell(E) \) is real analytic:

\[ S_\ell(E_-) = S_\ell(E_+^*) = S_\ell^*(E_+). \quad (5.3) \]

Let us define the scattering amplitude \( \mathcal{T}_\ell \) by

\[ S_\ell(E) = 1 + 2i \rho(E) \mathcal{T}_\ell(E). \quad (5.4) \]

The factor \( \rho(E) \) is of course arbitrary, and we will leave it so for the moment. A natural definition will arise below. The discontinuity relation for \( \mathcal{T}_\ell \) is:

\[ \mathcal{T}_\ell(E_+) - \mathcal{T}_\ell(E_-) = \rho(E_+) \mathcal{T}_\ell(E_+) \mathcal{T}_\ell(E_-). \quad (5.5) \]

**B. Threshold Branch Point.**

We can use this relation to deduce that it is possible to find a \( \rho(E) \) such that \( \mathcal{T}_\ell \) is two sheeted in the neighborhood of threshold.
Define $E_1$ to be a point in the scattering region and $E_n$ to be that point under $E_1$ obtained by circling threshold counter clockwise $(n-1)$ times. Equation (5.5) reads:

$$T_\ell(E_1) - T_\ell(E_2) = \rho(E_1) T_\ell(E_2) T_\ell(E_1).$$

Now continue the discontinuity relation once around threshold and obtain

$$T_\ell(E_2) - T_\ell(E_3) = \rho(E_2) T_\ell(E_3) T_\ell(E_2).$$

Eliminating $T(E_2)$ in order to get an expression for $T(E_3)$ in terms of $T(E_1)$

$$T_\ell(E_3) = \frac{T_\ell(E_1)}{1 + (\rho(E_1) + \rho(E_2)) T_\ell(E_1)}.$$ 

If $\rho(E)$ is chosen such that it changes sign upon circling the threshold branch point once, then $\rho(E_2) = -\rho(E_1)$, and $T_\ell(E_3) = T_\ell(E_1)$. Under these conditions $T_\ell(E)$ is two sheeted. The standard choices for the phase space factor $\rho$ are:

$$\rho_{\text{non-rel}} = q^{2\ell+1}, \quad \rho_{\text{rel}} = q^{2\ell+1}/E.$$ 

In terms of $q$ the relation $E_n \rightarrow E_{n+1}$ is just $q \rightarrow -q$. 
C. Second Sheet Structure.

The discontinuity relation, Eq. (5.5), gives the value of $T_{\ell}$ in the lower half $q$ plane in terms of $T_{\ell}$ in the upper half $q$ plane. And thus we are assured of the analytic structure of $T_{\ell}$ in the lower half plane (see Fig. 9b) in terms of the well known analyticity of the upper half plane. The kinematical branch point at $q = -i\pi$ for equal mass scattering for the relativistic amplitude comes from the phase space factor $\rho_{\text{rel}}$.

D. K Matrix.

The $K$ matrix can be defined which has better analyticity properties than $T_{\ell}$ and $S_{\ell}$ for our purposes.

\[ S_{\ell}(q) = \frac{1 + i\rho K_{\ell}(q)}{1 - i\rho K_{\ell}(q)} \quad (5.10) \]

Using continued unitarity, $S_{\ell}(q) = 1/S_{\ell}(-q)$, it follows that $K_{\ell}(q) = K_{\ell}(-q)$, and thus $K_{\ell}(q)$ is analytic in $q^2$ in the neighborhood of the origin. Fig. 10b shows the cut structure of $K_{\ell}(q)$ in the $E^2$ plane.
VI. SOLUTION OF THE BETHE-SALPETER DIFFERENTIAL EQUATION

Our calculation of phase shifts is done in two stages. First the partial wave amplitude is calculated at a set of energies below elastic threshold using a variational method based on the differential equation. The amplitude is then continued to the scattering region using the knowledge of its analytic structure dealt with in the previous sections. This section is devoted to the motivation for calculating below threshold and an outline of the methods used to calculate the input numbers for the continuation. We restrict ourselves to equal mass scattering.

A. Wick Rotation and Asymptotic Behavior.

The differential equation was solved for energy below threshold because only there is it simple to impose the boundary conditions on the wave function at infinity in coordinate space. The wave function is exponentially damped in this region and this is crucial for the application of our variational method.

The asymptotic behavior of the wave function can be found from the integral equation,\(^5\) (2.5). As long as the integral converges, we see that the large \(x\) behavior is governed by the free wave term and the Green's function. The free wave term can be easily subtracted out leaving the Green's function as our main concern.

It is well known that the Wick\(^6\) rotation can be performed on the Bethe-Salpeter equation for \(E\) below threshold. This can be best seen from the integral equation for \(T(k', k, E)\) in momentum space, Eq. (2.15). There are a multitude of singular surfaces adjacent to the
hypercontour in the real $p, p_0$ space. However, for $E^2 < (2m)^2$, there are no singularities in the first and third quadrants of the integration variable $p_0$ plane, for any value of $p$, and thus the contour can be rotated counter-clockwise by an angle $\pi/2$. The external momenta $k_0$ and $k'_0$ are also rotated and this operation transforms the equation to one in euclidean four-space. This will have the practical advantage of allowing the use of expansions in four dimensional spherical harmonics in the subsequent work. We will henceforth work with the rotated forms of the equations, where now all relative momentum vectors and coordinate vectors are euclidean:

$$k = (k, k_4) \quad x = (x, x_4),$$

$$k_4 = k_0 e^{-i\pi/2} \quad x_4 = x_0 e^{i\pi/2}.$$  \hspace{1cm} (6.1)

Turning now to the integral representation of the Green's function in $x$ space, Eq. (2.7), and holding $\omega^2 < m^2$, the Wick rotation can be carried out without passing any singularities. In the rotated form, the exponential components of the Green's function for large $x$ are:

$$G_K(x) \sim \exp[i \sqrt{\omega^2 - m^2} |x|] + \exp[i |x_4| - m R],$$

$$R = (|x|^2 + x_4^2)^{\frac{1}{2}}. \hspace{1cm} (6.2)$$

where $R = (|x|^2 + x_4^2)^{\frac{1}{2}}$. This clearly shows that for $\omega^2 < m^2$, the Green's function and hence the scattering part of the wave function is
exponentially damped in all directions of the euclidean four-space
\( (x, x) \), whereas for \( \omega^2 > m^2 \), the second term is a growing exponential
in \( x_4 \). This reflects the fact that poles of \( \tilde{\alpha}_K(p) \) have moved into
the first and third quadrants in Eq. (2.7) and have moved past the
rotated \( p_0 \) contour on the imaginary axis.

This shows that the Green's function is exponentially damped
for all \( \omega^2 < m^2 \). The scattered part of the wave functions is also
damped as long as the integral in Eq. (2.5) converges. For the off-mass-
shell case in which \( \omega \), and \( k \) are independent, the integral does
indeed converge for the full region of \( \omega \) stated. However, by going
to the mass shell, \( E^2 = 4(k^2 + m^2) \), below threshold the free wave
term \( \psi^0_K(x) \) in Eq. (2.5) becomes a real exponential and this competes
with the damped exponential under the integral giving only a finite
region of \( \omega \) where the scattered part of the wave function is exponen-
tially damped. It is this effect that signals the onset of the left
hand cut and will be discussed again below.

B. The Differential Equation.

We can obtain the differential equation from the integral
equation, Eq. (2.5), (where now all relative vectors are euclidean) by
operating on the equation with the differential operator with the
property

\[
\mathcal{G}(\partial_\mu) G(x - x') = \delta^4(x - x'), \tag{6.3}
\]

giving the wave function equation in the center of mass system:
where

\[ \mathcal{L}(\partial_\mu) \psi_{k,E}(x) = V(x) \psi_{k,E}(x) + \mathcal{L}(i \mathbf{k}_\nu) \psi_k^0(x), \quad (6.4) \]

and \( V(x) = I(x) \) expressed in the rotated variables. The last term comes from the free wave term in Eq. (2.5) and is zero for \( k_\nu \) on the mass shell.

Let us define the scattered part of the wave function by:

\[ \psi_{k,E}(x) = \psi_k^0(x) + \chi_{k,E}(x). \quad (6.7) \]

The differential equation for \( \chi_{k,E}(x) \) is:

\[ \mathcal{L}(\partial_\mu) \chi_{k,E}(x) = V(x) \chi_{k,E}(x) + \psi_k^0(x) V(x). \quad (6.8) \]

C. Variational Principle.

We can write a Kohn type variational principle based on the differential equation (6.8) that gives a stationary expression for \( T \):
It is easy to show that this expression is stationary with respect to first order variations of \( \chi_k(x) \) about its true solution, and thus a first order error in the wave function will give a second order error in \( T \).

\[
[T(k', k, E)] = \int d^4 x \: \chi_{k'}^* E (x) \sigma(\partial_x) - V(x) \chi_{k', E}(x) + \int d^4 x \: \chi_{k'}^* (x) V(x) \psi_k^0(x) + \int d^4 x \: \psi_k^0 (x) V(x) \chi_{k', E}(x)
+ \int d^4 x \: \psi_k^0 (x) V(x) \psi_k^0 (x).
\] (6.9)

It is easy to show that this expression is stationary with respect to first order variations of \( \chi_k(x) \) about its true solution, and thus a first order error in the wave function will give a second order error in \( T \).

\[
\frac{\delta[T]}{\delta \chi^*} = 0, \quad \frac{\delta[T]}{\delta \chi} = 0.
\] (6.10)

The last term of the variational principle is just the first Born term. This is considerably simpler to apply in practice than the Schwinger variational principle used by Schwartz and Zemach.\(^5\)

This variational principle is an exact statement and holds for arbitrary \( k, k', \) and \( E \). However, it may be that the integrals ostensibly diverge and must be defined by analytic continuation. Also when introducing a set of expansion functions for \( X \) which are capable of representing the true wave function it may well be that the matrix elements in such a basis will diverge. This happens for certain values of \( E, k, \) and \( k' \) and severely limits the applicability of this variational principle in practice. The off-mass-shell and on-mass-shell cases will be considered separately.
(i) Off-Mass-Shell.

For this case $E$ is independent of $k$ and $k'$. Fix $k$ and $k'$ to represent true scattering states: $k = (k_x, 0)$, $k' = (k'_x, 0)$, $|k| = |k'|$. For $E^2 < (2m)^2$, $\chi(x)$ is a decaying exponential for large $x$ and it may be represented well by a set of trial functions with a decaying exponential behavior and all the integrals in Eq. (6.9) converge. For $E^2 > (2m)^2$, however, $\chi(x)$ is a growing exponential in $x_4$ and it defies ones imagination to find a simple set of trial functions with the growing exponential that will yield convergent integrals. The derivative term in Eq. (6.9) is the troublesome one; all other terms have a potential present which is a decaying exponential in all directions. A possible method of circumventing this difficulty is to introduce an integral representation of the wave function

$$\chi_{k,E}(x) = \int d^4 x' \, C(x - x') \varphi(x').$$

An examination of the integral equation for $\chi(x)$ shows that $\varphi(x)$ contains a decaying exponential in the elastic scattering region. Using the property (6.3) the derivative term can be seen to be a convergent integral. But now we have integrals to evaluate of the same difficulty as the Schwinger method.5

(ii) On-Mass-Shell.

The additional constraints $E = \sqrt{(|k|)^2 + m^2} = \sqrt{(|k'|)^2 + m^2}$ limits further the applicability of Eq. (6.9). The free wave $\psi_k^0(x)$ which is oscillatory for the above case becomes a real exponential below
threshold and for \( \text{Im}(k) > \mu \), the integrals again diverge. Also at this point our estimate of the asymptotic behavior of \( \chi(x) \) is no longer valid as discussed above. So finally the domain of applicability in \( E \) is \( \frac{1}{4}(m^2 - \mu^2) < E^2 < (2m)^2 \). This is the region between elastic threshold and the second Born contribution to the left hand cut. (The first Born term was included explicitly.) These considerations might suggest that the full amplitude has a singularity at \( E^2 = \frac{1}{4}(m^2 - \mu^2) \). Although the variational principle for the full amplitude breaks down at this point, only the partial wave amplitude in fact has this singularity.

D. Numerical Method.

To solve the Bethe-Salpeter equation we first introduce a linear parameterization of the wave function \( \chi_k(x) \):

\[
\chi_k(x) = \sum_{\ell=0} a_{\ell, n, j} \left[ q_{n \ell 0} (\hat{x}) \varphi_j(R) \right],
\]

(6.11)

where \( q_{n \ell m} \) are four dimensional spherical harmonics on the four-sphere and \( \hat{x} \) is the unit four-vector in the euclidean space. The four dimensional spherical harmonics can be expressed in terms of the usual three dimensional spherical harmonics and Gegenbauer polynomials,

\[
c^\alpha_\beta \rightarrow 4 \cos \theta
\]

\[
q_{n \ell m}(\hat{x}) = Y_{n \ell m}(\hat{r}) \left[ \frac{2^{\ell+1}(n + 1)(n - \ell)! \ell!}{\pi (n + \ell + 1)!} \right]^{\frac{1}{2}} c^{\ell+1}_{n-\ell} (\cos \theta \cos \phi) \sin^\ell (\phi),
\]

(6.12)
where \( \cos \theta = \frac{x_\mu}{R} \), \( \hat{r} \) is the three-space unit vector and \( R \) is the length \( R = \left( |r|^2 + x_4^2 \right)^{\frac{1}{2}} \). The functions \( \varphi_j(R) \) are radial functions depending only on \( R \).

\[
\varphi_j(R) = R^j e^{-\alpha R}. \tag{6.13}
\]

We can expand \( X^*_k(x) \) in the same set of functions but now with expansion parameters \( b^j_{\ell',n',j'} \). These functions have been used before by Schwartz and have been taken over directly to our problem. The free wave term has the following expansion in this basis

\[
\psi^0_k(x) = (2\pi)^2 \sum_{n=0}^{\infty} \sum_{\ell=0}^{\infty} \frac{J_{n+1}(|k|R)}{|k| R} \sum_{m=-\ell}^{\ell} a_{\ell,n,m} \psi_{n,\ell,m}^*(\hat{k}) \psi_{n,\ell,m}(\hat{k}). \tag{6.14}
\]

where \( \hat{k} \) is the unit four vector in the direction \( k \) and \( |k| \) is its length, and \( J_n \) is the ordinary Bessel function.

Substituting these expansions in the variational principle, Eq. (6.9) and invoking the stationary condition:

\[
\frac{\delta S[T]}{\delta a_{\ell',n',j'}} = 0, \tag{6.15}
\]

we get linear equations for \( a_{\ell,n,j} \).

\[
\sum_{\ell=0}^{\infty} \sum_{n=\ell}^{\infty} \gamma_{\ell,n,j} a_{\ell,n,j} = \nu_{\ell',n',j'}, \tag{6.16}
\]

where
The ordinary angular momentum \( \ell \) is conserved and thus \( \mathcal{M}_{\ell', n'j', \ell n j} = M_{n'j', n j} \delta_{\ell'} \delta_{\ell} \). Equations (6.16) are inhomogeneous equations, the corresponding homogeneous equations are precisely the ones used by Schwartz for the bound state calculation of Reference 4. The new term \( V_{\ell n j} \) is:

\[
V_{\ell n j} = \frac{\hbar}{\hbar n 0(x)} \sqrt{4\pi(2\ell + 1)} \int_0^\infty dR R^{\ell+1} e^{-\alpha R} k_{\perp} (\mu R) J_{\ell+1}(|k|R).
\] (6.18)

Defining a partial wave amplitude

\[
T(k', k, E) = \sum_{\ell=0}^{\infty} (2\ell + 1) t_{\ell}(|k|, k_0, |k'|, k_0', q) P_{\ell}(\cos \theta),
\] (6.19)

where \( \cos \theta = \frac{k \cdot k'}{|k| |k'|} \), we obtain finally

\[
t_{\ell} = \sum_{n=\ell}^{\infty} a_{n l j}^* v_{n l j} + E_{\ell}(k', k_0', k, k_0),
\] (6.20)

where

\[
E_{\ell}(k', k_0', k, k_0) = \frac{\hbar^2 \lambda}{kk'} Q_{\ell} \left( \frac{k^2 + k'^2 - (k_0 - k_0')^2 + \mu^2}{2 kk'} \right),
\] (6.21)

and
The integrals for the matrix elements can all be done analytically and are described in Ref. 3. The integral for the vector term (6.18) was done numerically with a Laguerre integration formula. The recursion relation

$$J_{n-1}(z) + J_{n+1}(z) = \frac{2n}{z} J_n(z). \quad (6.23)$$

can be used for recursing down on the index $n$, and thus not all of the matrix elements need to be calculated from the integral.

We chose a sequence of trial functions letting $n = \ell, \ell + 1, \ldots, N$, and $j = n, n + 1, \ldots, N$ and increased $N$ to see convergence of our results. The parameter $\alpha$ was varied and chosen to be the value that gives the fastest convergence.

Table 2 gives some samples of convergence of $\tilde{t}_\ell = t_\ell - B_\ell$ for $S$ waves. Near threshold the convergence gets bad. For the on-shell case, near $E = 0$, the onset of the second Born contribution to the left hand cut, the convergence also deteriorates. In the neighborhood of a bound state which manifests itself as a pole in $t_\ell$, the convergence is also slower presumably because the pole position itself moves for successive approximations. Except for these special regions the convergence was good.
VII. ANALYTIC CONTINUATION TO THE SCATTERING REGION

The second step in calculating phase shifts is to continue the scattering amplitude to the physical region which is described in this section. The method of continuation is described in Appendix C. Below we discuss separately the off-mass-shell and on-mass-shell continuations. The latter method was more successful which was probably due to the fact that the function was smoother, i.e. there were fewer nearby singularities. Also the on-shell amplitude satisfies a simple unitarity constraint and this was used advantageously in the continuation.

A. Off-Mass-Shell Continuation.

Referring to Fig. 9a, we have as input for the continuation a set of values of \( t_\ell(k, 0, k, 0, q) \) for a set of values of \( q \) on the positive imaginary axis, for \( k \) fixed in the elastic scattering region. Our object is to continue \( t_\ell \) in \( q \) to the point \( q = k \). This function is meromorphic in the \( q \) plane in a convex region that contains the calculated points on the imaginary axis and the points of interest on the real axis. We set:

\[
t_\ell(k, 0, k, 0, q) = \frac{\sum_{i=0}^{N} a_i (-i^q)^i}{1 + \sum_{i=1}^{N} b_i (-i^q)^i} .
\]  

(7.1)

Since \( t_\ell \) is real on the imaginary \( q \) axis the coefficients \( \{a_i\} \) and \( \{b_i\} \) are real. We chose equal powers of \( q \) in numerator and denominator because \( t_\ell \to B_\ell \) as \( q \to \infty \). (The Born term \( B_\ell \) is independent
of \( q \).) The coefficients were determined using the methods of Appendix C. Finally we set \( q = k \) to get the phase shift from the expression

\[
t_{\lambda}(k, 0, k, 0, k) = \frac{8\pi E}{k} \frac{1}{A + i B},
\]

(7.2)

where

\[
A = \frac{\tan \delta}{k}, \quad B = 1 \text{ (unitarity)}.
\]

(7.3)

The accuracy in the calculated value of \( B \) serves as a check on the continuation.

The continuation was first done determining the coefficients by point-wise fitting, Eq. (C.5). For a moderately strong attractive potential with a deeply bound state \((\lambda = 3, \mu = m = 1)\), the results of the continuation were uncertain from 5% to 20% over the elastic region. A great many attempts were made to improve this. These included:

(a) determining the coefficients by more sophisticated methods (see Appendix C),
(b) varying the distribution of input points,
(c) trying to improve the accuracy of input numbers,
(d) putting known singularities in the fitting functions,
(e) generating a power series for \( t_{\lambda} \) in \( q \) and then forming true Padé approximants and
(f) continuing in the internal masses. No significant improvement was achieved. The Schrödinger equation was solved by Schlessinger and Schwartz very successfully using this method.\(^{25}\) There are two principle differences between these two problems: (1) The Bethe-Salpeter amplitude has an
infinite number of branch points on the real axis. These include the normal thresholds and a host of others due to our choice of off-mass-shell variables. The Schrödinger amplitude is of course regular on the real $q$ axis. (2) The Bethe-Salpeter equation is two dimensional in $|x_2|$ and $x_4$, compared to the one dimensional Schrödinger radial equation. This fact limits the accuracy which is practical to achieve using the Kohn method. Since simplicity was a desirable element in this calculation, we felt that it would be self defeating to attempt a more sophisticated solution of the equation.

Figure 11 gives our results where the errors bars indicate the approximate uncertainty in the phase shift. The dotted line gives the values taken from the Schwartz and Zemach calculation. We used twenty input points in the bound state region between $q = 0$ and $q = 3i$, and used the Legendre fit, Eqs. (C.12).

It may appear wasteful of computer time in that the function must be calculated at many points to get the phase shift at one point. However, it should be noticed in Eq. (6.16) that $k$ appears only in the inhomogeneous term and after calculating and inverting the matrix $M$ which depends on $E$ its inverse can be applied to vectors $V$ with different values of $k$ which uses a small fraction of computer time. The continuation time itself is very small.

B. On-Mass-Shell Continuation.

Because of the dubious success of the off-mass-shell continuation a search was made for a smoother function with fewer nearby singularities. The study of the singularity structure of amplitudes leads us to believe that the on-shell $K$ matrix is the optimum function.
As shown in Sec. V, \( K(E^2) \) is analytic in \( E^2 \) at threshold and has branch points only on the real \( E^2 \) axis, (see Fig. 10).

The calculation proceeds as follows: \( t_\ell(q) \) (suppressing the first four arguments) is calculated as described in Sec. VI where

\[
t_\ell(q) = B_\ell(q) + \tilde{t}_\ell(q).
\]

The first born term \( B_\ell(q) \) is known exactly and \( \tilde{t}_\ell(q) \) is calculated numerically. Substituting Eq. (6.20) in Eq. (7.3), \( K(E^2) \) can be found for \( 4(m^2 - \mu^2) < E^2 < 4m^2 \). It is a real analytic function of \( E^2 \) with a branch point at \( E^2 = 4m^2 - \mu^2 \) coming from \( B_\ell(q) \). We can then expand the domain of analyticity further by removing the cut contribution to \( K(E^2) \) for \( 4(m^2 - \mu^2) < E^2 < 4m^2 - \mu^2 \). Define:

\[
\tilde{K}_\ell(E^2) = K(E^2) - K^\text{cut}(E^2),
\]

where

\[
K^\text{cut}(E^2) = \frac{1}{\pi} \int_{4(m^2 - \mu^2)}^{4m^2 - \mu^2} dE^2 \frac{\Delta K(E^2)}{E^2 - E^2},
\]

and

\[
\Delta K(E^2) = \frac{1}{2i} (K(E^2 + i\epsilon) - K(E^2 - i\epsilon)).
\]
The function \( \tilde{\kappa}_f(E^2) \) is analytic on the real axis in the region
\[ 4(m^2 - \mu^2) < E^2 < (2m + \mu)^2. \]
This function was continued to the scattering region using the Legendre fit, Eq. (C.12), in the variable \( E^2 \), and then the cut contribution \( \kappa_f^{\text{cut}}(E^2) \) was added back in. The phase shift was found from the formula:

\[
\kappa_f(E^2) = \frac{4\pi E}{k} \tan \delta_f. \tag{7.9}
\]

The results compared quite favorably with the Schwartz and Zemach results for moderately strong potentials. The relative errors in the phase shifts for various potentials are plotted in Fig. 12. In the region of \( E^2 \) between zero and four, the relative error of \( \tilde{\kappa}_f \) is plotted. We see that on the average about two significant digits are lost in the extrapolation. The error increases for stronger potentials.

C. Comparison.

A comparison of the results calculated in these two ways serves to point out the fact that the continuation will be more successful when there are fewer nearby singularities to contend with. As explained in Appendix C the Padé approximants represent branch cuts by a line of poles. It is important to get a good representation of the function for lower orders of fitting functions because cancellations in the fitting procedure limits the practical number of fitting parameters for the accuracy of our input numbers. Also convergence or stability of the extrapolated numbers must be observed upon increasing the number of parameters.
We can estimate from considering Fig. 9a that at least four poles are necessary to represent the nearby cuts of the off-shell amplitude. This means nine parameters in our functions. Whereas the nearby cuts in the on-shell amplitude \( \tilde{\mathcal{K}}(E^2) \), Eq. (7.4), could probably be represented by two poles (Fig. 10b). The presence of bound states of course further increases the number of poles necessary to get a good representation. For stronger potentials the input numbers are less accurate, there are more nearby bound state poles, and the discontinuities across the nearby cuts are larger.
VIII. VARIATIONAL CALCULATION OF REGGE TRAJECTORIES IN POTENTIAL THEORY

A method for calculating Regge trajectories also developed out of this study of variational principles and analytic properties. Again, the calculation was set up for \( E \) below threshold, but for this problem it was found that the variational equations themselves could be continued to arbitrary energies. This method has the three virtues of being simple fast and accurate on an electronic computer. It has been used extensively for the study of the superposition of two Yukawa potentials \(^43\) and has also been generalized to the two channel problem. \(^44\)

A. The Bound State Problem.

Let us start from a consideration of the bound state problem for physical \( \ell \). For our conventions the Schrödinger equation is

\[
(H_{\ell} - \ell^2) \psi(x) = 0, \tag{8.1}
\]

where

\[
H_{\ell} = -\frac{1}{r^2} \frac{d}{dr} r^2 \frac{d}{dr} + \frac{\ell(\ell + 1)}{r^2} + V. \tag{8.2}
\]

The bound state eigenvalue problem is determined by boundary conditions for large and small \( r \). For small \( r \), the wave function is controlled by the angular momentum barrier with the two possible behaviors:

\[
\psi_1 \sim r^\ell, \quad \psi_2 \sim r^{-(\ell+1)} \text{, for } r \to 0. \tag{8.3}
\]
For large $r$, the $k^2$ term is most singular and two independent solutions are

$$
\psi_1' \sim e^{ikr}, \quad \psi_2' \sim e^{-ikr}, \text{ for } r \to \infty. \quad (8.4)
$$

The bound state wave function must satisfy the boundary conditions $\psi_1$ and $\psi_1'$, which is possible for isolated values of $k^2$.

The Rayleigh-Ritz variational method provides a good way to find the eigenvalue,

$$
[k^2] = \frac{\int_0^\infty r^2 \, dr \, \varphi_\ell \, H_\ell \, \psi_\ell}{\int_0^\infty r^2 \, dr \, \varphi_\ell \, \psi_\ell}. \quad (8.5)
$$

This gives $k^2$ as a functional of the wave function, stationary about the true eigenstate. Let us expand the wave function in terms of the following basis functions with linear variational parameters.

$$
\psi_\ell = 2\beta \sum_{n=0}^N a_n (2\beta r)^{n+\ell} \, e^{-\beta r}, \quad (8.6)
$$

with a similar expansion for $\varphi_\ell$ with coefficients $b_n$. These trial functions are good representations of the wave function in that they have a power series expansion about the origin starting with the power $\ell$ and are exponentially damped at infinity. These functions can have at most $N$ nodes and therefore can represent at most $N + 1$ bound states. The variable $\beta$ is not treated as a variational parameter at this point but will be chosen as dictated by the asymptotic behavior.
Substituting these expansions in the variational principle
Eq. (8.4) and invoking the stationary condition
\[ \frac{\delta S[k^2]}{\delta b_n} = 0, \quad (8.7) \]
we get the equations
\[ \sum_n (H_{mn} - k^2 I_{mn}) a_n = 0, \quad (8.8) \]
where
\[ H_{mn} = (2\beta)^2 \int_0^\infty r^2 \, dr \, (2\beta r)^m \, e^{-\beta r} \int_0^\infty r^2 \, dr \, (2\beta r)^n \, e^{-\beta r}, \quad (8.9) \]
and
\[ I_{mn} = (2\beta)^2 \int_0^\infty r^2 \, dr \, (2\beta r)^m \, e^{-\beta r} \int_0^\infty r^2 \, dr \, (2\beta r)^n \, e^{-\beta r}. \quad (8.10) \]
Equation (8.8) is of course just the Schrödinger equation in this basis.
We consider potentials of the form
\[ V(r) = \sum_{s=1}^p \lambda_s \frac{e^{-\mu_s r}}{r}. \quad (8.11) \]
Equations (8.8) have solutions when
\[ \det |H_{mn} - k^2 I_{mn}| = \mathcal{P}(k, \ell, (\lambda_s, \mu_s), \beta) = 0. \quad (8.12) \]
The explicit forms of these matrices are

\[ H_{mn} = \beta^2 \Gamma(2\ell + m + n - 1) \left[ 4\ell(\ell + 3/2) - (m - n)^2 + m + n \right] \]

\[ + 2\beta \Gamma(2\ell + m + n) \sum_{s=1}^{P} \lambda_s \left( \frac{2\beta}{2\beta + \mu_s} \right)^{2\ell + m + n}, \]  

(8.13a)

and

\[ I_{mn} = \Gamma(2\ell + m + n + 1). \]  

(8.13b)

Thus to find an eigenvalue \( k^2 \), pick a value of \( \beta \), search for a zero of \( F^N \), take a sequence of values of \( N \) and examine convergence. In practice the eigenvalue converges independently of the value of \( \beta \), but the rate of convergence can be considerably enhanced by a good choice of \( \beta \). For \( -k^2 \) not too small and for a single attractive Yukawa potential, the accuracy is about one significant digit per trial function for the ground state.

B. Continuation in \( \ell \).

The continuation to arbitrary complex \( \ell \) is immediate. The Regge continuation is defined by making \( \ell \) complex and maintaining the boundary condition \( \psi \to r^\ell \) as \( r \to 0 \). A study of the equation for small \( r \) shows that the wave function has a power series expansion starting with \( r^\ell \), i.e. \( \psi_\ell \sim r^\ell (c_0 + c_1 r^+ \ldots) \). Our trial functions have just this behavior. The matrix elements contain gamma functions of non-integer argument, but there are no other changes.
It should be pointed out that for \( \text{Re}(\ell) < -\frac{1}{2} \), the variational principle is not well defined. This is because the numerator integral of Eq. (8.14) diverges at its lower limit in that region. The denominator integral diverges for \( \text{Re}(\ell) < -\frac{3}{2} \). However, these integrals define analytic functions of \( \ell \) for \( \text{Re}(\ell) > -\frac{1}{2} \). Their values to the left of \( \ell = -\frac{1}{2} \) can be defined by analytic continuation. These integrals are of the form:

\[
I(a) = \int_{0}^{\infty} x^a f(x) \, dx, \quad (8.14)
\]

where \( f(x) \) has a power series expansion about the origin and goes to zero at infinity faster than any power. This integral is defined for \( \text{Re}(a) > -1 \). Integrating by parts \( N \) times and fixing \( \text{Re}(a) > -1 \) we find

\[
I(a) = (-)^N \int_{0}^{\infty} dx \frac{x^{a+N} F^{(N)}(x)}{\prod_{i=1}^{N} (a + i)}. \quad (8.14')
\]

The condition on "a" allowed us to throw away the boundary contributions. However, this integral is now defined for \( \text{Re}(a) > -N - 1 \). There are clearly poles in "a" which accounts for the divergence of the integral (8.14). This is the unique analytic continuation to the left of \( a = -1 \).

The matrix elements (8.9), (8.10) are also of the form (8.14). Since we can do the integrals explicitly we can analytically continue the results to any value of \( \ell \). The gamma functions have poles that account for the divergences discussed above.
C. Continuation in $E$

This method is applicable as it stands to all values of $k$ where the trial functions can represent the true wave function. Since the Regge pole wave function has an asymptotic behavior $e^{ikr}$ for large $r$, we see that for $\text{Im}(k) > 0$, the wave function is damped exponentially for large $r$ and thus the above method is applicable in the upper half $k$ plane. On the real $k$ axis the wave function oscillates asymptotically and thus the method breaks down. For $\text{Im}(k) < 0$, the method a fortiori breaks down since the wave function grows exponentially there.

These regions can be made accessible to this method using a trick due to Regge. The point is that the contours of the integrals in Eq. (8.5) can be rotated by an angle $\theta, \theta < \pi/2$,

$$r' = r e^{-i\theta}, \quad (8.15)$$

without passing singularities or picking up end point contributions provided the potential has no singularities in $r$ in the region swept out by the rotation. For a finite superposition of Yukawa potentials this condition is satisfied. For $\theta > \pi/2$, the potential will grow exponentially for large $r$. We solve the Schrödinger equation in the rotated coordinate $r'$:

$$\left[ -e^{-2i\theta} \frac{1}{r'^2} \frac{d}{dr'} r'^2 \frac{d}{dr'} + e^{-2i\theta} \frac{\ell(\ell + 1)}{r'^2} + V(e^{i\theta} r') - k^2 \right] \psi(r') = 0. \quad (8.16)$$
Multiplying through by \( e^{2i\theta} \) we obtain the original equation in the new coordinate where the only changes are the potential \( \tilde{V} = e^{2i\theta}V(r'e^{i\theta}) \) and the energy \( \tilde{E} = k^2 e^{2i\theta} \). The asymptotic behavior of the wave function is now \( \exp(i k \exp(i \theta) r') \) for large \( r' \). We have rotated the half \( k \) plane where the wave function is exponentially damped and thus have a new region where our method is applicable. The changes in the above formulae are trivial. The Regge trajectories are now solutions to the equation:

\[
\tilde{F}^N(k e^{i\theta}, \lambda, [\lambda_s e^{i\theta}, \mu_s e^{i\theta}], \beta) = 0. \tag{8.17}
\]

The calculation proceeds as follows: choose an energy \( k \) and an appropriate angle \( \theta \) such that the true wave function is exponentially damped. Then search for a zero of \( \tilde{F}^N \) as a function of \( \lambda \). Look at a sequence of \( N \)'s and examine convergence. A reasonable choice of \( \beta \) is

\[
\beta = A \text{Im} (k e^{i\theta}), \quad A \approx 1 \text{ to } 3.
\]

The convergence is excellent except in the neighborhood of \( k = 0 \). This is because the true asymptotic behavior of the wave function has not been included properly. This can be more or less serious depending on how much structure the trajectory has for small \( k \). Figure 13 shows the leading trajectory in the region near \( k = 0 \) for a strong attractive potential with a long range repulsion for different
values of $\beta$. All curves would converge to the curve $\beta_3$ with a sufficient number of trial functions. For this case eleven trial functions were used. This potential has an $S$ wave resonance and its position and width can be calculated accurately with eleven trial functions.
IX. SUMMARY AND CONCLUSIONS

We have presented methods in this thesis which use analytic properties of solutions in conjunction with variational principles for solving off-shell equations. For the Bethe-Salpeter calculation of phase shifts, the equation was solved in the region where it was most readily done, and then the phase shifts were found by numerical analytic continuation. For the potential theory calculation of Regge trajectories again the calculation was set up in the most advantageous region and then the equations themselves were continued to any desired region. In both cases a knowledge of the analytic structure of the continued function was necessary.

Continuation of the variational equations themselves is superior to numerical continuation, but we feel that the latter method can have its place in future calculations. As more difficult problems are attempted, it is natural to try to solve the bound state problem first and one of the most economical and efficient ways is with the Rayleigh-Ritz technique. The subsequent calculation of the T matrix in the bound state region can be carried out by merely introducing an inhomogeneous term to the homogeneous bound state equations. Then at least scattering lengths and effective ranges can be calculated by numerical analytic continuation.

Because of the dubious success of the off-mass-shell continuation over a large energy range, it is clear that more work is necessary to make this method generally acceptable. If more of the nearby singularities could be removed or included properly, the method would probably work better. By going to the mass-shell, we were able to remove one
branch point and put others in advantageous places. The mass-shell method has certain disadvantages though. If we introduce a superposition of potentials, the accessible region where the equation can be solved is between threshold and the second Born contribution to the left hand cut of the longest range component of the potential. For complicated potentials this could be a severe limitation.

Interesting possibilities are suggested by the Regge trajectory calculation. We were able to do the calculation in regions of angular momentum where the original variational principle was undefined, i.e., where the integrals diverged. This was possible because we knew the detailed behavior of the wave function at the origin and built it in to our trial functions. If we could do the same thing for the boundary condition at infinity it would be possible to continue the equations to values of energy where the integrals diverged. This will be more difficult because the wave function has an essential singularity at infinity for both the Schrödinger and Bethe-Salpeter cases. For the Regge pole calculation presented here, we could get to any desired value of energy by going to a complex coordinate, but this trick would not work for a scattering state wave function and has not yet been generalized to the Bethe-Salpeter equation.
I am pleased to thank Professor Charles Schwartz for suggesting this problem and for his guidance and encouragement. I am also indebted to Professor Charles Zemach for initiating my work on the Bethe-Salpeter equation which led to this research, and to Leonard Schlessinger for helpful discussions on the numerical continuation procedure. I would also like to express my appreciation to William Kaufmann and Klaus Rothe for many discussions throughout the course of this work.

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APPENDIX A. DISCONTINUITY FORMULA

In this appendix we show what kind of branch point is produced by the pinching of two branch points in a single integral of the form:

\[ f(z') = \int_{\Gamma} dz' g(z - z') h(z - a), \quad (A.1) \]

where \( \Gamma \) is shown in Fig. 14 and where \( g(z) \) and \( h(z) \) have branch points at \( z = 0 \). The integral \( f(z') \) can have a branch point at \( z' = a \) arising from the pinch of these two branch points under the integral. We will give a formula for its discontinuity in terms of the discontinuities of the two pinching branch points.

Distorting the contour around the branch point at \( z = a \) as shown in Fig. 14b,c, we can write

\[ f(z') = \int_{\Gamma'} dz' g(z - z') h(z - a) + 2i \int_{\Gamma'} dz' g(z - z') \Delta h(z - z), \quad (A.2) \]

where

\[ \Delta h(z - a) = \frac{1}{2i} (h(z - a + i\epsilon) - h(z - a - i\epsilon)). \quad (A.3) \]

We have assumed that the integral on the small circle around the branch point at \( z = a \) is zero. For the case of a branch point off the real axis we define the discontinuity of a function \( f(z) \) with a branch point at \( z_0 \) to be
\[ \Delta f(z) = \frac{1}{2\pi i} (f(z) - f(\tilde{z})) \]  

(A.4)

where \( \tilde{z} \) is that point under \( z \) found by circling the branch point once in the counterclockwise direction. This corresponds to the earlier definition for \( z_0 \) real and the cut drawn to the right.

The discontinuity of \( f(z') \) is given by the difference of the integrals depicted in Fig. 14b and Fig. 14c. The integral over \( \Gamma \) drops out in the difference and the result is

\[ \Delta f(z') = 2i \int_{a}^{z'} dz \Delta g(z - z') \Delta h(z - a). \]  

(A.5)

The pinching of two logarithmic branch points, \( g(z) = h(z) = \log(z) \), for example gives a branch point whose discontinuity is \( \Delta f(z') = 2i \pi^2 (z' - a) \).
APPENDIX B. ELASTIC THRESHOLD BRANCH POINT

In this appendix we will prove that the elastic threshold branch point of the partial wave Bethe-Salpeter amplitude is two sheeted in $\omega^2$ for both legs off the mass-shell. In Sec. V we showed that this is the case for the on-shell amplitude. It is implicit in the paper of Levine et al.\textsuperscript{6} that the singly off-shell $T$ matrix has this property. We will generalize this result to the doubly off-shell $T$ matrix following the methods of Kowalski.\textsuperscript{46}

It can be shown that each term in the Born series is two sheeted at threshold (except the first which is independent of $\omega^2$) and if the Born series converges, then it follows that the partial wave amplitude is also two sheeted. We prefer to work with the integral equation for the sake of elegance so as not to have to rely on the convergence of the Born series.

Following the conventions of Sec. IV, Levine et al.\textsuperscript{6} defined a new function $f_\epsilon$ through the equation:

$$T_\epsilon(k', k'_0, q, 0, \omega) = f_\epsilon(k', k'_0, q, 0, \omega) T_\epsilon(q, 0, q, 0, \omega).$$  \hspace{1cm} (B.1)

The function $f_\epsilon$ clearly has the property:

$$f_\epsilon(q, 0, q, 0, \omega) = 1. \hspace{1cm} (B.2)$$

Substituting this in the Bethe-Salpeter equation, we arrive at a formula for the on-shell $T$ matrix.
where all arguments except $q$ are suppressed for fully on-shell quantities.

The integral equation for $f_{\ell}$ is

$$f_{\ell}(k', k'_0, q, 0, \omega) = \frac{B_{\ell}^{(1)}(k', k'_0, q, 0)}{B_{\ell}^{(1)}(q)}$$

$$+ 1 \int_0^\infty dp \int_{-\infty}^\infty dp'_0 \mathcal{M}(k'_0, k, p, p'_0, \omega) \mathcal{G}(p, p'_0) f(p, p'_0, q, 0, \omega),$$

where

$$\mathcal{M}(k'_0, k', p, p'_0, \omega) = \frac{B_{\ell}^{(1)}(k', k'_0, q, 0) B_{\ell}^{(1)}(p, p'_0, q, 0)}{B_{\ell}^{(1)}(q)} - B_{\ell}^{(1)}(k', k'_0, p, p'_0).$$

The advantage of introducing the function $f_{\ell}$ is that it does not have a threshold branch point as we will show; the $T$ matrix is calculated through the formulae (B.3) and (B.1), the branch point coming from a pinch in the integral.

Consider an integral of the form

$$I = \int_0^\infty dp \int_{-\infty}^\infty dp'_0 \mathcal{E}(p, p'_0) \mathcal{G}(p, p'_0).$$
where \( E_{q}(p, p_0) \) is even in \( p \), which allows us to symmetrize the \( p \) integration and the function \( E \) depends only on \( q^2 \) in the neighborhood of threshold. The integrals (B.3) and (B.4) are of this form. This follows from the fact that \( X_{q}(k', k_0', k, k_0, \omega) = (-)^{l+1} X_{q}(-k', k_0', k, k_0, \omega) \) where \( X_q \) is \( T, f, M \) or \( B^{(1)} \). The same relation holds for the right leg. The Green's function has four poles in the \( p_0 \) plane—two in the upper half and two in the lower half. The \( p_0 \) contour is on the real axis. Distort the contour into the upper half plane as shown in Fig. 15a to \( p_0 \) picking up the residues of the poles. The integral can be written:

\[
I = \int_{-\infty}^{\infty} dp \int_{\Gamma_{p_0}} dp_0 \left\{ \frac{E(p, \omega - \sqrt{p^2 + m^2})}{\omega - \sqrt{p^2 + m^2}} + \frac{E(p, -\omega - \sqrt{p^2 + m^2})}{\omega + \sqrt{p^2 + m^2}} \right\}. \tag{B.7}
\]

The integral along \( p_0 \) experiences no pinches and is regular at \( \omega^2 = m^2 \). The integrand of the \( p \) integral has singularities at \( p = \pm q \) as shown in Fig. 15b. The pinching between these two poles gives the threshold branch point at \( q = 0 \). Passing the \( p \) contour to \( \Gamma_{p} \) (Fig. 15b) we arrive at

\[
I = \int_{-\infty}^{\infty} dp \int_{\Gamma_{p_0}} dp_0 + \int_{\Gamma_{p}} dp + \frac{m}{8\pi^2 \omega q^2} E(q, 0). \tag{B.8}
\]
The first two integrals are regular in \( q^2 \) at threshold and the second integral is \( q \) times an even function of \( q \), thus exhibiting the two sheeted branch point.

The considerations apply for Eq. (B.3) and the Born series of Sec. IV. However, for the integral equation for \( f_\ell \), (B.4), \( E(q, 0) = 0 \). The function \( M \) has zeros just so as to kill the poles that produce the pinches and thus \( f \) will have no threshold branch point.

The generalization to both legs off the mass-shell has been carried out by Kowalski for the Schrödinger equation and generalizes immediately to the Bethe-Salpeter equation. The generalized form of Eq. (B.1) is

\[
T_\ell(k', k_0', k, k_0, \omega) = f_\ell(k', k_0', q, 0, \omega) T_\ell(q) f_\ell(k, k_0, q, 0, \omega)
\]

\[\quad + f_\ell(k', k_0', k, k_0, \omega) B_\ell^{(1)}(q) - f_\ell(k', k_0', q, 0, \omega) B_\ell^{(1)}(k, k_0, q, 0).\]  

This reduces to Eq. (B.1) for the right leg on mass-shell. For the left leg only on-mass-shell we obtain

\[
f_\ell(q, 0, k, k_0, \omega) = \frac{B_\ell^{(1)}(k, k_0', q, 0)}{B_\ell^{(1)}(q)}. \tag{B.10}
\]

Note that \( f_\ell \) is not symmetric in its right and left legs.

The arguments go through just as before: Eq. (B.9) gives the off-shell T matrix in terms of the on-shell T and \( f \), Eq. (B.3) still gives the on shell T in terms of \( f \), but the integral equation for \( f \) is now:
\[
\begin{align*}
  f_{\ell}(k', k'_0, k, k_0, \omega) &= \frac{\mathcal{B}_{\ell}(1)(k', k'_0, k, k_0)}{\mathcal{B}_{\ell}(1)(q)} \\
  &+ i \int_0^\infty dp \int_{-\infty}^\infty dp_0 \ M(k', k'_0, p, p_0, \omega) \ G_{\omega}(p, p_0) \ f(p, p_0, k, k_0, \omega).
\end{align*}
\]
Our method requires the use of numerical analytic continuation. We chose to do this using a ratio of polynomials for fitting functions. This is the form of a Padé approximant, though we do not determine the coefficients of the polynomials in the canonical way. We find empirically that our fitting functions have properties very similar to Padé approximants and thus it is worthwhile to mention some of the rudimentary facts about Padé approximants because they serve as a guide line in determining the expected region of convergence.\textsuperscript{47,48}

Consider a function defined by a power series with a finite radius of convergence.

\[ f(z) = \sum_{i=0}^{\infty} a_i z^i. \quad (C.1) \]

Suppose we would like to evaluate the function outside the circle of convergence at a point \( z' \). One way to do this is to determine the function and all its derivatives at a new point \( z \) within the circle of convergence and thus define a new power series in \( (z - z_0) \) that has a new circle of convergence and in this way progress to the desired point \( z' \) to evaluate the function. This is very hard to do in practice because each coefficient of the new power series in \( (z - z_0) \) is itself a power series in \( z_0 \) which converges slowly for large \( z_0 \).

However, if the point of interest \( z' \) lies within any circle that includes the origin and excludes all singularities, then there is
a much better way to evaluate the function at \( z' \). We can map an arbitrary circle in the \( z \) plane containing the origin into a circle in the \( w \) plane with center at the origin using the fractional linear transformation that preserves the origin,

\[
z = \frac{Aw}{1 - Bw}. \tag{C.2}
\]

All interior points of the circle in the \( z \) plane are mapped into interior points in the \( w \) plane. Substituting Eq. (C.2) in Eq. (C.1) and expanding out the denominators we generate a power series in \( w \). The transformations can be chosen such that \( w' \) will lie in the circle of convergence of the \( w \) plane where

\[
w' = \frac{z'}{A + Bz'}. \tag{C.3}
\]

Similarly we can map circles in the \( z \) plane that exclude the origin onto circles centered at the origin in the \( w \) plane using the transformation (C.2) but now the exterior of the circles in the \( z \) plane gets mapped into the interior of the circles in the \( w \) plane. Thus finally we can evaluate the function in this way at any point that lies inside a circle that includes the origin and excludes all singularities and at any point that lies outside a circle that excludes the origin and includes all singularities. We call this region \( R \).

Pade approximants are rational approximations to the function defined from a power series that are invariant under the transformation (C.2). The \([M, N]\) Pade approximant is defined formally
\[
[M, N] (z) = \frac{\sum_{i=0}^{M-1} b_i z^i}{1 + \sum_{i=1}^{N-1} c_i z^i} = \sum_{i=0}^{J} a_i z^i, \quad (C.4)
\]

where \( M + N = J + 2 \). The coefficients \( b_i \) and \( c_i \) are determined by demanding that the power series expansion of the ratio of polynomials coincides with the power series expansion on the right for the first \( J \) terms. This yields linear equations for \( \{b_i\} \) and \( \{c_i\} \) as can be seen from the equivalent procedure of multiplying the denominator through and comparing powers of \( z \).

The invariance of Padé approximants under the fractional linear transformation \((C.2)\) means that it will have the same value at a point \( z' \) when derived from the power series in \( z \) as at the point \( w' \) \((Eq. (C.3))\) when derived from the corresponding power series in \( w \).

And thus if the Padé approximants converge within the circle of convergence in the \( z \) plane, they will necessarily converge in the region \( R \).

The theory of convergence of Padé approximants as \( M = N + K \to \infty \), \( K \) fixed is incomplete as discussed in Ref. 47. For functions that go to a constant at infinity just such a sequence for \( K = 0 \) is needed. The utility of Padé approximants to us lies in whether or not they converge rapidly for small orders and provide an economical and stable sequence of approximations, and this can only be decided empirically. We will state though the conjectured domain of convergence which is a liberal estimate that will in particular be a guide as to where we do not expect convergence.
Conjecture: At least a subsequence of Padé approximants \([M, N](z)\) converges as \(M = N + K \to \infty\), \(K\) fixed, in a domain \(\tilde{R}\) defined as the union of the interior of all circles that contain the origin and exclude all non-polar singularities and the exterior of all circles that exclude the origin and include all non-polar singularities, excluding in addition small circles around each pole.

Comments: \(\tilde{R}\) differs from \(R\) in that poles are allowed in the domain \(\tilde{R}\). This is because poles arise naturally from zeros in the denominator, but since the function goes to infinity in the neighborhood we exclude small circles around each pole. For a multisheeted function the domain \(\tilde{R}\) defines a single sheet as illustrated in Fig. 16. Convergence is slower near these "natural cuts" because presumably the poles of the Padé approximants will lie along the cuts.

For our applications we know the function at a set of points rather than a power series. We still use the Padé form but determine the coefficients by constraining the two forms to be equal at the input points. The equations to determine \((b_i)\) and \((c_i)\) are

\[
\left(1 + \sum_{i=1}^{N-1} c_i z^i \right) f(z) = \sum_{i=0}^{M-1} b_i z^i. \tag{C.5}
\]

where \(s = 1, 2, \ldots, M + N - 1\). This method of computing the coefficients is the simplest. However, if the function is given at \(J\) points there are a large number of ways to choose \(j\) of them for \(j < J\) and thus there is no well defined sequence for judging the convergence of the approximations.
An improvement on this method is to introduce a set of \( J \) linearly independent weight functions \( W_j(z) \) and solve the following equations:

\[
\sum_{i=1}^{N-1} c_i z_s^i f(z_s) - \sum_{i=0}^{M-1} b_i z_s^i \right) = 0.
\]

where \( j = 1, 2, \ldots, M + N - 1 \). A sequence of weight functions (e.g. \( W_j(z) = z^j \)) determines a sequence of approximations. This has the advantage of using all the input points for each approximation. For \( j = J \) this is equivalent to Eqs. (C.5) because then \( W_{js} = W_j(z_s) \) is a square nonsingular matrix and we get Eqs. (C.5) by multiplying Eqs. (C.6) by \( w^{-1} \). Equations (C.6) reduce identically to Eqs. (C.5) if \( W_j(z_s) = \delta_{js} \).

A special case of Eq. (C.6) is a least square fit upon introducing the weight functions

\[
W_j(z) = \begin{cases} -U(z) z^j & j = 1, \ldots, N-1, \\ U(z) z^j & j = N, \ldots, (M+N-1). \end{cases}
\]

Substituting this in Eq. (C.6) we get the conditions for a minimum of the expression:

\[
\gamma = \sum_s U(z_s) \left( 1 + \sum_{i=1}^{N-1} c_i z_s^i \right) f(z_s) - \sum_{i=0}^{M-1} b_i z_s^i \right)^2 = 0.
\]
The function $U(z_s)$ is an arbitrary function that can be chosen to weigh accurate points more heavily than inaccurate points.

Another special case of Eq. (C.6) that has nice algebraic properties is the weight function

$$W_j^j(z_s) = P_j(z_s) V_s$$

where $P_j$ are Legendre polynomials, and $z_s$ and $V_s$ are the Gaussian $J$ point integration quadrature points and weights. In addition let us write the polynomials in the Padé quotient as Legendre polynomials.

$$f(z) = \frac{\sum_{i=0}^{M-1} b_i P_i(z)}{1 + \sum_{i=1}^{N-1} c_i P_i(z)}$$

Now the sum over $z_s$ becomes an integral

$$\sum_{s=1}^{J} V_s g(z_s) = \int_{-1}^{+1} dz \ g(z)$$

and we get the following equations

$$M_0 + \sum_{i=1}^{N-1} M_i c_i^i = \sum_{i=0}^{M-1} N_i b_i^i,$$

where

$$M_j^i = \int_{-1}^{+1} dz \ P_j(z) f(z) P_i(z),$$
and

\[ N_{j1} = \int_{-1}^{+1} P_j(z) P_1(z) = \frac{281j}{2j + 1}. \]  \hspace{1cm} (C.14)

The recursion relation

\[ (1 - 1)(2j - 1) M_{ij,j} = (2j - 3) M_{i,j+1} \]

\[ - (2j - 1)(1 - 2) M_{j-2,j} + (2j - 3)(j - 1) M_{i-1,j} \]  \hspace{1cm} (C.15)

enables one to calculate all matrix elements in terms of the matrix elements of the first row and last column.

The equations (C.12) are very similar in form to the equations for true Padé approximants (C.4). The coefficients of true Padé approximants are obtained by comparing powers of \( z \) and Eqs. (C.12) are obtained by comparing coefficients of Legendre polynomials. Of course any set of orthogonal polynomials can be used that are appropriate for the particular problem.

One further remark to be made is that the numerator and denominator functions need not be polynomials but can be any sequence of functions with linear parameters. For example it might be desirable to put in known branch points with an appropriate choice of functions. In addition the sequence of functions in the numerator need not be the same as the denominator.
1. G. F. Chew, The Analytic S Matrix, (W. A. Benjamin, Inc., New York, 1966); The basic philosophy of S matrix theory is presented here and in Ref. 2.
13. C. Lovelace, Phys. Rev. 135, B1225 (1964); Further references are given here.
15. C. Schwartz (private communication).
29. This was carried out for the full Bethe-Salpeter amplitude in Ref. 23.
30. This method has been partially generalized to the Bethe Salpeter equation by W. Kaufmann. (paper in progress)
34. A good account is given in Ref. 2.

35. See Ref. 2 for example pages 65 and 118.

36. Ibid, p. 64.

37. Ibid, p. 57.


39. R. C. Hwa and V. L. Teplitz, Homology and Feynman Integrals, (W. A. Benjamin Inc. New York, 1966); See also Ref. 2.

40. See Ref. 2. The content of this section is a review of well known properties of unitarity.

41. See Ref. 5, Sec. IV.C.

42. Our formulas are taken from M. Abramowitz and I. Stegun, Handbook of Mathematical Functions (Dover Publications, Inc., New York, 1965). Some formulae are given concisely in Ref. 4.


44. Work in progress by N. Bali and the author.


49. See Ref. 42, Sec. 25.
TABLE 1. Singular surfaces of the Bethe-Salpeter second Born term $B_{k}^{(2)}(k', k', k, k_0, \omega)$ classified according to the number of singular surfaces, $S_1 = 0$, of the integrand participating.

<table>
<thead>
<tr>
<th>No. of Surfaces</th>
<th>Singular Surfaces Participating in Integrand</th>
<th>Singular Surface in Integral</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$S_1, S_2, S_3, S_4$</td>
<td>$\mu^2 = 0$</td>
</tr>
<tr>
<td></td>
<td>$S_5, S_6$</td>
<td>$\sigma^2 = 0$</td>
</tr>
<tr>
<td>2</td>
<td>$S_1 S_2, S_3 S_4$</td>
<td>$(k-k')^2 - (k_0 - k'_0)^2 + 4\mu^2 = 0$</td>
</tr>
<tr>
<td></td>
<td>$S_1 S_4, S_2 S_3$</td>
<td>$(k+k')^2 - (k_0 - k'_0)^2 + 4\mu^2 = 0$</td>
</tr>
<tr>
<td></td>
<td>$S_5 S_6$</td>
<td>$\sigma^2 = \mu^2$</td>
</tr>
<tr>
<td></td>
<td>$S_1 S_5, S_2 S_5$</td>
<td>$k^2 - (k_0 - \omega)^2 + (\mu + m)^2 = 0$</td>
</tr>
<tr>
<td></td>
<td>$S_1 S_6, S_2 S_6$</td>
<td>$k^2 - (k_0 + \omega)^2 + (\mu + m)^2 = 0$</td>
</tr>
<tr>
<td></td>
<td>$S_3 S_5, S_4 S_5$</td>
<td>$k'^2 - (k'_0 - \omega)^2 + (\mu + m)^2 = 0$</td>
</tr>
<tr>
<td></td>
<td>$S_3 S_6, S_4 S_6$</td>
<td>$k'^2 - (k'_0 + \omega)^2 + (\mu + m)^2 = 0$</td>
</tr>
</tbody>
</table>

(Table 1 continued)
<table>
<thead>
<tr>
<th>No. of Surfaces</th>
<th>Singular Surfaces Participating in Integrand</th>
<th>Singular Surface in Integral</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>$S_1 S_5 S_6, S_2 S_5 S_6$</td>
<td>$((k-q)^2 - k_0^2 + \mu^2)((k+q)^2 - k_0^2 + \mu^2) = 0$ \ (10)</td>
</tr>
<tr>
<td></td>
<td>$S_3 S_5 S_6, S_4 S_5 S_6$</td>
<td>$((k'-q)^2 - k'_0^2 + \mu^2)((k'+q)^2 - k'_0^2 + \mu^2) = 0 \ (11)$</td>
</tr>
<tr>
<td></td>
<td>$S_1 S_3 (S_5), S_2 S_4 (S_5)$</td>
<td>$[ (k'^2 - (k_0 \omega)^2 + \mu^2 - m^2)(k_0 \omega) - (k'^2 - (k_{0} \omega)^2 - \mu^2 - m^2)(k_0 \omega) ]^2$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$- [ (k'^2 - (k_0 \omega)^2 + \mu^2 - m^2) k - (k'^2 - (k_0 \omega)^2 + \mu^2 - m^2) k' ]^2$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$+ 4 [ k' (k_0 \omega) - k (k_0 \omega) ]^2 m^2 = 0 \ (12)$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Equation (12) with $k \rightarrow -k \ (13)$</td>
</tr>
</tbody>
</table>

Equation (12) with $k \rightarrow -k$
TABLE 2. Sample of convergence of the variational calculation of
\[ \tilde{t}_q(k, 0, k, 0, q) \]
for \( \lambda = 3, \mu = m = 1, \ell = 0 \). (a) off-shell, \( k^2 = 0.4m^2 \). (b) on-shell \( k^2 = (E^2/4) - m^2 \). For both cases, the convergence is better for weaker potentials and for repulsive potentials. The sign change is due to a bound state at \( E^2 \approx 1 \).

<table>
<thead>
<tr>
<th>Dim</th>
<th>( E^2 = 3.8603 )</th>
<th>( E^2 = 2.8165 )</th>
<th>( E^2 = -0.870615 )</th>
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<tr>
<td></td>
<td>( \alpha = 0.35 )</td>
<td>( \alpha = 0.9 )</td>
<td>( \alpha = 2.2 )</td>
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<td>-626.6</td>
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<td>-474.1</td>
<td>-733.28</td>
<td>608.182</td>
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<td>6</td>
<td>-470.7</td>
<td>-708.67</td>
<td>707.085</td>
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<td>9</td>
<td>-444.3</td>
<td>-702.01</td>
<td>723.856</td>
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<tr>
<td>12</td>
<td>-444.1</td>
<td>-698.42</td>
<td>727.655</td>
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<tr>
<td>16</td>
<td>-435.7</td>
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<td>20</td>
<td>-434.9</td>
<td>-696.93</td>
<td>728.079</td>
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<tr>
<td>25</td>
<td>-431.4</td>
<td>-696.77</td>
<td>728.086</td>
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<tr>
<td>36</td>
<td>-429.3</td>
<td>-696.60</td>
<td>728.095</td>
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</tbody>
</table>

(Table 2 continued)
On-shell $\tilde{t}(q,0,q,0,q)$

<table>
<thead>
<tr>
<th>Dim</th>
<th>$E^2 = 3.5$</th>
<th>$E^2 = 2.0$</th>
<th>$E^2 = 0.5$</th>
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<td>$\alpha = 0.7$</td>
<td>$\alpha = 1.3$</td>
<td>$\alpha = 1.1$</td>
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<td>2</td>
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<td>4</td>
<td>-761.9</td>
<td>-2148.71</td>
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<td>6</td>
<td>-752.9</td>
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<td>12</td>
<td>-732.5</td>
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<td>16</td>
<td>-729.4</td>
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<td>-728.2</td>
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<td>-727.5</td>
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<td>-727.1</td>
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</tr>
<tr>
<td>36</td>
<td>-726.9</td>
<td>-2006.59</td>
<td>7048.7</td>
</tr>
</tbody>
</table>
TABLE 3. Samples of the stability of the extrapolation for the off-mass shell continuation (a), and the on-mass-shell continuation (b). The S. Z. values are taken from the Schwartz and Zemach calculation\(^5\) (private communication). For both cases, \(\mu = 1\).

(a) Off-shell Continuation

<table>
<thead>
<tr>
<th>Padé Approximant</th>
<th>(\lambda = 1, E^2 = 4.4)</th>
<th>(\lambda = 1, E^2 = 5.6)</th>
<th>(\lambda = 3, E^2 = 5.2)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Unitarity</td>
<td>(\delta_0/\pi)</td>
<td>Unitarity</td>
</tr>
<tr>
<td>2, 2</td>
<td>0.979</td>
<td>0.526</td>
<td>1.091</td>
</tr>
<tr>
<td>3, 3</td>
<td>0.978</td>
<td>0.528</td>
<td>1.085</td>
</tr>
<tr>
<td>4, 4</td>
<td>1.049</td>
<td>0.496</td>
<td>0.972</td>
</tr>
<tr>
<td>5, 5</td>
<td>1.107</td>
<td>0.515</td>
<td>0.966</td>
</tr>
<tr>
<td>6, 6</td>
<td>1.079</td>
<td>0.495</td>
<td>0.976</td>
</tr>
<tr>
<td>7, 7</td>
<td>1.026</td>
<td>0.512</td>
<td>0.970</td>
</tr>
<tr>
<td>8, 8</td>
<td>1.064</td>
<td>0.506</td>
<td>0.971</td>
</tr>
<tr>
<td>S. Z.</td>
<td>1.0</td>
<td>0.49865</td>
<td>1.0</td>
</tr>
</tbody>
</table>

(b) On-shell Continuation

<table>
<thead>
<tr>
<th>Padé Approximant</th>
<th>(\lambda = 3, E^2 = 5.6) ((\delta_0/\pi) - 1)</th>
<th>(\lambda = 0.7, E^2 = 5.2)</th>
<th>(\lambda = -1, E^2 = 4.4)</th>
</tr>
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<tbody>
<tr>
<td>2, 2</td>
<td>-0.2420</td>
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<td>0.2674</td>
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<td>4, 4</td>
<td>-0.3277</td>
<td>0.2672</td>
<td>-0.13623</td>
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<tr>
<td>5, 5</td>
<td>-0.3048</td>
<td>0.2666</td>
<td>-0.13625</td>
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<td>6, 6</td>
<td>-0.3083</td>
<td>0.2670</td>
<td>-0.13623</td>
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<td>7, 7</td>
<td>-0.3095</td>
<td>0.2663</td>
<td>-0.13631</td>
</tr>
<tr>
<td>8, 8</td>
<td>-0.3119</td>
<td>0.2731</td>
<td>-0.13626</td>
</tr>
<tr>
<td>S. Z.</td>
<td>-0.3097</td>
<td>0.2684</td>
<td>-0.13610</td>
</tr>
</tbody>
</table>
Fig. 1. Diagrammatic representation of the inhomogenous scattering equation.
Fig. 2. Complex planes pertinent to the Schrödinger second Born term. Poles are marked by a cross and branch points with a dot with arbitrary trailing cuts. (a) Singularities of the integrand of Eq. (3.7) in the integration variable, p, plane. (b), (c) Singularities of $B_2^2(k', k, q)$ in the k and q planes respectively.
Fig. 3. Complex planes pertinent to the Schrödinger third Born term corresponding to Fig. 2 for the second Born term. There is in addition a branch point at \( q = -i\mu/2 \).
Fig. 4. The box diagram and some pertinent contracted diagrams with singularities independent of $\cos \theta$. The sheet structure of singularities for cases (c) and (d) are shown.
Fig. 5. (a) The N-rung Feynman ladder diagram. (b) A possible contracted graph with the $M^\text{th}$ inelastic threshold.
Fig. 6. (a) Some singular surfaces of the integrand for the Bethe-Salpeter second Born term $B_\ell(2)$ ($k', k_0', k, k_0, \omega$) for $\omega^2 > m^2$. $S_2$, $S_3$ and $S_4$ were left out for the sake of clarity. (b) Singularities of (a) in the $p_0$ complex plane for fixed real $p$. 
Fig. 7. Some singularities of the Bethe-Salpeter second Born term \( B_2^{(2)}(k', k_0', k, k_0, \omega) \) as a function of the left leg variables \( k', k_0' \). The subscripts on \( T \) refer to the surfaces \( S_i \) that are responsible for it. The disappearance of a three-surface singularity \( T_{156} \) on other sheets of two-surface singularities \( T_{15} \) and \( T_{16} \) is shown. For the case drawn, \( m^2 < \omega^2 < (m + \mu)^2 \). The surfaces given by Eqs. (3), (4) of Table 1 were omitted for the sake of clarity. The singularities given by Eqs. (12) and (13) do not intersect the real \( k', k_0' \) plane for the right leg variables \( k, k_0 \) chosen. (b) \( k_0' \) plane for \( k' \leq q \).
Fig. 8. Singularities of the Bethe-Salpeter second Born term in the $q$ plane for $k_0 = k'_0 = 0$. (a) $k = k'$ fixed in the scattering region. (b) $k = k' = q$. 
Fig. 9. Important singularities of $B^N(k',k'_0,k,k_0,\omega)$ in the $q$ plane for $k_0 = k'_0 = 0$, in the variables of Fig. 8. (a) The normal thresholds lie on the positive and negative real $q$ axis. There are many more singularities than just normal thresholds on the real axis, e.g. the surface $T_{1,3,5}$ of Fig. 8 and its offspring in higher Born terms for $q$ sufficiently larger than $k$. There are also branch points at $q = -\sigma \mu/2, \sigma = 1,2,\cdots,(N-2)$. 

(b) In the on-mass-shell variable $q = k = k'$, only normal thresholds are on the real axis. $T_i$ is the $i$th threshold.
Fig. 10. (a) Definition of $E_+$ and $E_-$ for defining continued unitarity.
(b) Cut structure of $K(q)$ in the $E^2$ plane for the Bethe-Salpeter amplitude showing the first inelastic threshold and the first two contributions to the left hand cut.
Fig. 11. S wave phase shifts in the elastic region calculated using the off-mass-shell continuation (solid curve) with estimated error bars. The dotted curves were taken from Schwartz and Zemach. The masses are $m = \mu = 1$.5
Fig. 12. Relative errors incurred in the calculation of phase shifts using the on-mass-shell continuation. The variational calculation was done in the region $0 < E^2 < 4$ and the errors indicate the quality of the input numbers for the extrapolation. The extrapolated region is for $E^2 > 4$. 
Fig. 13. Real and imaginary parts of the leading Regge trajectory versus energy for 11 trial functions for different $\beta$'s, where $\beta$ is the exponential parameter in the trial function. The value of $\bar{\beta}$ was chosen to be $\text{Im}(k e^{i\theta})$. All curves would converge to the one labeled $\beta_3$ upon increasing the number of trial functions.
Fig. 14. Relevant complex planes for the discontinuity formula of Appendix A.
Fig. 15. Contour distortions for integrations generating the threshold branch point by pinching of Green's function poles.
Fig. 16. Examples of conjectured convergence domain $\tilde{R}$ for Padé approximants (unshaded area), $B$, $P$, $C$ stand for branch point, pole and center of power series. The shaded region indicates schematically regions of slower convergence.
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