Bifunctionate Solutions to the Schrödinger Equation for Reactive, Three-Atom, Collinear Encounters.

Thesis by

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In Partial Fulfillment of the Requirements

for the Degree of

Doctor of Philosophy

California Institute of Technology

Pasadena, California

1973

(Submitted May 8, 1973)

Abstract

Two methods for solving the Schrödinger equation for one dimensional, three atom, electronically adiabatic, reactive collisions have been investigated. The first bifunctionate method was proposed by Diestler in 1969. It solves for vibrational excitation probabilities by expanding two parts of the total solution to the scattering problem in eigenfunctions of the unperturbed diatoms. These diatoms are the target and product diatoms in the reactive encounter. This formalism allows the eigenfunction series representation of the total solution to decay to zero in the interaction region of the reaction. Proposition 1 shows that this decay process is indicative of a failure in Diestler's method which renders its solutions invalid.

A technique proposed as a means of solving the equations governing nuclear collisions was also investigated. This formalism, called the Method of Subtracted Asymptotics, has been shown to be an application of the general mechanism of eigenfunction expansion to the scattering problem. Because of analysis problems induced by the extensive eigenfunction series demanded by this method, the Method of Subtracted Asymptotics is not an efficient or practical manner of solving the scattering problem. This method is treated in part 2 of this work.

Tests used to varify the numerical accuracy of several studies of the Method of Subtracted Asymptotics required the values of several special functions on the complex plane. To

meet these needs, algorithms which compute the value of a complex number raised to a complex power, the Gamma function, the Digamma function and the Hypergeometric function were prepared. These algorithms are discussed and presented in part 1 of this thesis.

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Introduction

The primary domain of this thesis is reactive, collinear, electronically adiabatic, atom-diatom scattering. The central goal of the numerical methods discussed in part two in this work is the solution of the collinear scattering equations. The complex functions of part one solve the Schrödinger equation for a central, one dimensional barrier and two of the five propositions which end this work support portions of the material in parts one and two.

There are, however, a few segments of this thesis which extend beyond the bounds of scattering theory. Appendix A of part one presents a representation of the Hypergeometric function which is of no utility in scattering studies and this appendix is therefore mathematics for mathematic's sake. Several of the propositions are far removed from scattering theory. They represent personal interests of the author.

Mathematical studies of quantum phenomena in reactive scattering were initiated in the 1960's. Primarily, these studies were undertaken because computers at last made the calculations possible. A further motivation for this work was the need to resolve the question of the applicability of classical mechanics to chemical reactions. Quantum mechanics describes all particle reactions correctly but it is a very intractable means by which to do so. Hence, if quantum mechanics can be approximated by classical mechanics for most atom reactions, a great

deal of complexity in the calculations can be avoided. A significant number of trajectory studies on model surfaces existed before quantum calculations were undertaken so comparson between quantum results and classical results for identical systems depended solely on obtaining the quantum data. The bulk of the work reported in this thesis was aimed at clarifying quantum mechanical methods by which one could create quantum, reactive, cross sections.

A number of systems which are currently the focus of intense experiments await elucidating contributions from quantum, reactive scattering calculations. Several studies at present appear to indicate that quantum phenomena control a major segment of the physics of the three atom reactions. Thus, in molecular beam studies, for example, classical mechanical models such as "stripping" and "harpooning" will not yield a valid understanding of the processes leading to the final observed cross sections. Quantum studies will probably be needed to elucidate the physics of gas flow chemilluminescence reactions. Vibrational and rotational populations in lasers will also require quantum treatment if current indications of failure by classical mechanics for these systems are confirmed.

Before quantum mechanics can be fully applied to realistic systems, questions about the validity of electronic adiabaticity, one dimensional atom impact and other approximations must be answered. This study did not aid in the verification of the

limits of classical mechanics nor did it test any of the dubious approximations of quantum mechanics. Instead, the material contained herein serves to remove two specious approaches to the answers to these problems.

Part I

Special Functions On The Complex Plane

Introduction

The solutions to most ordinary and partial differential equations are not simple rational functions of the equation variables. Instead, a small group of the solutions to differential equations can be represented as limited or infinite expansions and most solutions exist only as a numerical table of function values. Those functions which solve a differential relationship and can be expressed in some closed form have been termed special functions.

A large number of special functions are in common use in scattering theory. The Hermite polynomials, Legendre polynomials, the Laguerre polynomials and the spherical harmonics are all special functions which are basic to descriptions of quantum scattering phenomena (Ey44). In the following five sections, a group of special functions of a more limited applicability to scattering phenomena are discussed and algorithms for preparing values of these functions are presented.

All of these functions are prepared over their most general range, the complex field. In section 1, the complex power function is described. The Gamma function is discussed in section 2 and its logarithmic derivative, the Digamma function, is treated in section 3. Two forms of a hypergeometric function comprise sections 4 and 5. A representation of Gauss' series, a hypergeometric function, for the unit circle of the complex plane is the subject of section 4 while section 5 displays the formulas

needed to analytically continue Gauss' series to the entire complex plane.

These functions are all parts of the solution to the problem of scattering from an Eckart barrier (Ec30). This barrier along the x axis has the functional form,

$$V(x) = \frac{A e^{2\pi x/\ell}}{1 + e^{2\pi x/\ell}} + \frac{B e^{2\pi x/\ell}}{(1 + e^{2\pi x/\ell})^2} \qquad (1)$$

where ℓ is the width of the barrier and A and B are constants.

The one dimensional Schrödinger equation for a particle encountering this central potential is

$$\left[\partial^2/\partial x^2 + 2m/\hbar^2 \left\{ \frac{A z}{(1 - z)} + \frac{B z}{(1 - z)^2} + E \right\} \right] \Psi = 0$$

where $z = -e^{2\pi x/\ell}$. Transforming to the z plane gives

$$\left\{ z^2 \partial^2/\partial z^2 + z \partial/\partial z + 2m\ell^2/\hbar^2 \left[\frac{A z}{1 - z} + \frac{B z}{(1 - z)^2} + E \right] \right\} \Psi = 0. \qquad (2)$$

If Ψ is taken to be

$$\Psi = z^p (1 - z)^q F(\alpha, \beta; \gamma; z),$$

then equation 2) can be written

$$\partial/\partial z \left[z \Psi' \right] = \Psi (1 - z)^{-1} \left[-2m\ell^2/h^2 (A - E) - \frac{2m\ell^2 E}{(h^2 z)} - \frac{2m\ell^2 B}{h^2 (1 - z)} \right]. \qquad (3)$$

Ey44 Henry Eyring, John Walter, George E. Kimball, Quantum Chemistry, Chapter 4, John Wiley and Sons, New York, (1944).

Ec30 Carl Eckart, The Penetration of a Potential Barrier by Electrons, Physical Review, 35, #11, 1303, (1930).

Sn52 Chester Snow, Hypergeometric and Legendre Functions with Applications to Potential Theory, page 5, equation 12, National Bureau of Standards, Applied Mathematics Series, Vol. 19, (1952).

By comparing terms between equation 3) and the general hypergeometric equation form (Sn52)

$$\partial/\partial z\left[z^{\gamma-2p}(1-z)^{\alpha+\beta-\gamma+1-2q}\Psi' \right] = \Psi z^{\gamma-2p-1}(1-z)^{\alpha+\beta-\gamma-2q}* \left[(p+q-\alpha)(p+q-\beta) + \frac{p(\gamma-1-p)}{z} + \frac{q(\alpha+\beta-\gamma-q)}{1-z} \right], \quad (4)$$

the six equations which define the parameters of the solution $\Psi(z)$ can be distinguished.

$$z = -e^{2\pi x/\ell} \quad (5a)$$

$$\gamma - 2p = 1 \quad (5b)$$

$$\alpha + \beta - \gamma - 2q = -1 \quad (5c)$$

$$(p+q-\alpha)(p+q-\beta) = C(A-E) \quad (5d)$$

$$p(\gamma-1-p) = CE \quad (5e)$$

$$q(\alpha+\beta-\gamma-q) = CB \quad (5f)$$

Here, C is defined by $C = -2m\ell^2/h^2$ and h is Planck's constant.

The Eckart barrier problem of equation 2) was solved both numerically and analytically. The hypergeometric function algorithm of sections 4 and 5 was prepared to check the results of the computer program which numerically integrated equation 2). The other algorithms were created to supply function values needed in calculating $F(\alpha, \beta; \gamma; z)$.

All of the algorithms presented here have been prepared in the computer language Fortran IV. The programs were run on the model 360-75 and the model 370-155 I. B. M. computers under release 20.7.

I. Complex Numbers Raised to an Arbitrary Complex Power

If x and y are real numbers, the number x^y is a well defined real number. On the complex plane, this specificity disappears and, if a branch cut is not imposed, the combination of complex numbers

$$P(z_1, z_2) = z_1^{z_2} \tag{1}$$

is not well defined.

The ambiguity of the results of the operation of a complex exponent is one example of a general phenomenon in complex functions. Most functions on the complex plane are multiply valued. Their answers are not completely fixed by the specification of the initial data.

This arbitrariness in complex arithmetic is caused by the closure properties of the complex set. The set of complex numbers normally used in complex arithmetic can be represented by

$$C_0 = \{z \mid z = re^{i\theta}, \ -\pi < \theta \leq \pi\} \tag{2}$$

where a specific range has been chosen for the variable θ. When a function operates on an element of C_0, it relates one element of the range of the function, C_0, to an element of the domain of the function, D. The problem of closure associated with this process is that the elements contained in D for a multiple-valued function will not all be elements of C_0. Some of the elements of D will have a θ argument that will exceed the bounds of C_0 and thus the function is not closed over its range.

Most techniques for closing a function on the complex set cause uniqueness problems in the action of the function. These uniqueness difficulties will be displayed by using the branch cut technique on the power function. The definition of the power function, $P(z_1, z_2)$ is

$$P(z_1, z_2) = z_1^{z_2} = e^{z_2 \text{Log}_e z_1} \tag{3}$$

Example 1: Calculate the value of $(i^{10})^{1/10}$.

In the real plane, $(x^y)^{1/y} = x$. The following calculation will show that this pattern of behavior is not followed in a complex, branched plane.

From (I 3)

$$i^{10} = e^{10 \text{Log } i} = e^{10[\text{Log}_e 1 + \pi/2i]}$$

$$= e^{5\pi i}.$$

This intermediate result

$$i^{10} = e^{5\pi i} \tag{4}$$

shows why the definition of a branch on the complex spiral does not remove all the difficulties encountered with the function P. The complex number, $e^{5\pi i}$, is not in the set of all complex numbers

$$C_0 = \{z \,|\, z = r\, e^{i\theta},\ -\pi < \theta \leq \pi\},$$

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* The definition of the complex logarithm is $\text{Log}_e z = \ln r + i\theta$, $z = re^{i\theta}$.

even though the two input terms to P, i and 10, are members of this set. Thus, the function P is not closed over the set C_0.

The result, $e^{5\pi i}$, is usually represented as being in the set C_0. Thus, it is calculated modulo 2π and gives

$$e^{5\pi i} = e^{i\pi}. \tag{5}$$

The problem has been reduced to $(e^{i\pi})^{1/10}$ and an additional application of P gives

$$(e^{i\pi})^{1/10} = e^{\log(-1)/10} = e^{\pi i/10}$$

$$= \cos \pi/10 + i \sin \pi/10$$

$$= .9511 + .0390\ i.$$

Therefore, for the real numbers, x and y

$$P(P(x, y),\ 1/y) = x$$

but

$$P(P(i, 10),\ 1/10) = .9511 + .3090\ i.$$

This calculation shows that the use of a branch cut for complex calculation does not give all of the properties that are desired in an arithmetic. However, virtually all work with complex functions is done with the aid of a branch cut and virtually all computer representations of complex numbers impose a branch cut. The problems of phase specific answers and multiple roots which occur for the power function when it is used with a branch cut are the reason that such a basic routine is not already in existence.

When faced with the problem of establishing a function which mathematically might never give the specific answers wanted, compiler programmers abandoned the area of complex arithmetic to the user. Since the ability to raise a complex number to a complex power was fundamental to all work done on the complex plane, an algorithm based on the [x, y] complex arithmetic of the FØRTRAN language was prepared. The routines of algorithm 1a and 1b calculate all answers in in the C_0 set. Hence, the branch cut problems aluded to in Example 1 must be corrected by the user.

Mathematical Method:

The value of the complex number $z_1^{z_2}$ is calculated by

$$z = e^{(z_2 * \log(z_1))} .$$

This routine follows the convention that zero to the zero power equals 1.

$$0.0^{0.0} = 1.0$$

Possible Errors:

Because of magnitude limitations on the exponential function, the modulus of $z_2 * \log(z_1)$ should be less than 175.

$$|z_2 * \log(z_1)| < 175.0$$

Accuracy:

All calculations indicate that 6-digit or 12-digit accuracy are maintained by the single and double precision routines, respectively.

II. The Gamma Function

The Gamma function is a generalization of the factorial function

$$f(n) = n! = 1*2 \ldots *n, \qquad (1)$$

and it extends the definition of the factorial to all non-integer numbers of the complex plane. There are several representations for $\Gamma(z)$ (3), but the function is usually defined by the integral relation

$$\Gamma(z) = \int_0^\infty e^{-\tau} \tau^{z-1} \, d\tau \qquad \text{Real } (z) > 0. \qquad (2)$$

The Gamma function is a single valued, analytic function on the complex plane. Thus, it requires no branch cut for its implementation. The function has a pole at all negative integers and the origin.

Mathematical Method:

Two series representations are used to calculate the value of the Gamma function in the two unit wide strip about the imaginary axis defined by

$$-1 \leq \text{Real}(z') \leq 1. \qquad (3)$$

All arguments are reduced to this strip by the use of the recursion relations:

$$\Gamma(z+n) = z*(z+1)*..*(z+n-1)*\Gamma(z) \qquad \text{Real}(z) \geq 0.0 \qquad (4)$$

or

$$\Gamma(z-n) = \Gamma(z)/(z-1)*(z-2)*\ldots*(z-n) \qquad \text{Real}(z) < 0.0 \, . \qquad (5)$$

When equations II 4) or II 5) have reduced the complex

variable, z, to its equivalent value within the domain of equation II 3), the imaginary portion of the variable is used to select which of the two series will be used to calculate the function.

Let the equivalent value of z within the domain of equation II 3) be called z′. The imaginary part of z′ defines the two domains,

Domain 1

$$|\text{Imaginary}(z')| < 3.4 \tag{6}$$

and

Domain 2

$$|\text{Imaginary}(z')| \geq 3.4, \tag{7}$$

which are the zones of validity of the two series representations of $\Gamma(z)$.

Within domain 1, the 26-term power series developed by Davis (1), (2), is used to calculate the Gamma function. The series form is

$$1/\Gamma(z) = \sum_{i=1}^{26} a_i z^i \tag{8}$$

where the a_i are monotonically decreasing functions of i. All coefficients are listed, with references, in (2).

Domain 2 can be considered the asymptotic region of the Gamma function and, therefore, an asymptotic expansion (4) of the function is used to calculate $\Gamma(z)$ when z′ is in this region. Up to 26 terms of the asymptotic form

$$\ln \Gamma(z') \cong (z' - \tfrac{1}{2}) \ln z' + \tfrac{1}{2} \ln (2\pi) - z' + \sum_{m=1}^{\infty} B_{2m} / [2m(2m-1) z'^{(2m-1)}] \qquad (9)$$

$$|\arg z'| < \pi$$

may contribute to the preparation of the value of the function. The Bernoulli numbers, B_{2m}, used in this series are listed to 15 digit accuracy in Table I.

Possible Errors:

The use of the power series expansion to calculate $\Gamma(z)$ can cause underflows for values of z within a radius of 10^{-3} of any positive integer on the real axis.

Overflows may result if the argument passed to the algorithm has a magnitude greater than 60. Such arguments give results which are too large to be represented on most computers.

A call to the program generating the Gamma function which passes a negative integer or zero to the program will cause the printing of an error message. The function will return the value $\Gamma(z) = 1.0 \times 10^{65} + 0.0i$ upon receiving a non-positive integer argument.

Accuracy:

The accuracy of this algorithm has been tested by comparison to the tables of reference (2). The accuracy of these routines is not constant across the entire complex plane but, in general, single precision results were found to match published data to 6 significant figures while double precision

results duplicated published results to 10 significant figures.

As the value of the function argument, z, moves away from the real axis, the accuracy of all results decreases to a minimum and then returns to the accuracy noted above. The minimum in the accuracy of this algorithm occurs at

$$|\,\text{Imaginary}(z)\,| = 3.39\ .$$

The sixth digit of the values returned by both routines begins to differ from published values when

$$|\,\text{Imaginary}(z)\,| \cong 2.5\ .$$

At the value $|\text{Imaginary}(z)| = 3.3\overline{9}$, the values returned by the algorithm are only valid to 4 significant figures. Beyond $|\text{Imaginary}(z)| = 3.3\overline{9}$, the accuracy of the results increases until, at $|\text{Imaginary}(z)| = 4.0$, the general comments made above concerning accuracy are again applicable.

Relation to Factorial Notation:

The relationship between the Gamma function and the more common factorial notation is:

$$\Gamma(n+1) = n! \quad n \text{ integer},\ n \geq 0.$$

III. The Psi Function

The Logarithmic Derivative of the Gamma Function

The appearance of a particular combination of functions in the results of several diverse areas of mathematics often results in the definition of a label which can be used to denote the particular function combination every time it appears. The Psi function is such a label and its notation, $\psi(z)$, is used to denote a combination of Gamma functions.

The Psi function is also known as the logarithmic derivative of the Gamma function and the Digamma function. The definition of $\psi(z)$ is:

$$\psi(z) = d/dz\ [\text{Log}_e\ \Gamma(z)] = \Gamma'(z)/\Gamma(z) \quad . \tag{1}$$

Equation (III 1) explains why $\psi(z)$ is called the logarithmic derivative of the Gamma function. Its name, "Digamma Function," comes from the series of functions created by taking $n^{\underline{th}}$ order derivatives of $\log_e \Gamma(z)$. This series of functions is called the Polygamma function ladder and $\psi(z)$ is the first of these functions.

As is generally true of derivatives, $\psi(z)$ is less well behaved than its integral. In the region, Real $(z) > 0$, $\psi(z)$ is a monotonically increasing function of z. Beyond the point $z = 1$, the rate of increase of this function becomes very small.

However, in the half plane, Real $(z) \leq 0.0$, the function resembles cotan (πz) and possesses poles at all non-positive integers on the real axis. This behavior of the function dictated that an asymptotic expansion be used to represent the function.

The Psi function is a single-valued, analytic function on the principal value, complex plane, C_0. Therefore, no branch cut is needed to define $\psi(z)$.

Mathematical Method

Calculations for any argument are carried out in the complex half plane, Real (z) $\geq$ 5.0. Here, the asymptotic expansion:

$$\psi(z) = \mathrm{Log}_e\, z - 1/(2z) - \sum_{n=1}^{\infty} B_{2n}/(2nz^{2n}), \qquad (2)$$

holds. The constant B_{2n} is the Bernoulli number of order 2n. A compilation and discussion of Bernoulli numbers will be found in (5). However, a more accurate calculation of these figures has been carried out and the results are listed in Table 1.

If the argument passed to the routine is such that Real (z) $<$ 0, the reflection formula

$$\psi(1-z) = \psi(z) + \pi \cot(\pi z) \qquad (3)$$

is used to move the calculation into the positive Real (z) half plane.

Should the argument received through a call to the routine or the argument developed by the use of equation (III 3) lie in the region,

$$0 \leq \mathrm{Real}(z) < 5,$$

the recursion relation

$$\psi(z+1) = \psi(z) + 1/z \qquad (4)$$

is used to move the argument into the asymptotic region Real(z) $\geq$ 5.0, of the half plane, Real (z) $>$ 0, where equation (III 2) holds.

Possible Errors

The ψ function is highly oscillatory in the half plane, Real (z) ≤ 0. A request for the value of $\psi(z)$ at a point in this half plane may result in an underflow or overflow. Further, the ψ function has poles at all negative integers and zero. A call for the value of $\psi(z)$ at a non-positive integer will result in the printing of an error message. The value returned for $\psi(z)$ at such a point is

$$\psi(z) = 1.0 \times 10^{65} + 0.0\ i.$$

Accuracy

The algorithm used to create the value of $\psi(z)$ has been found to be accurate to six significant figures when calculated in single precision arithmetic. Values were checked against data compiled by Davis (1).

A double precision form of this algorithm was found to match compilations currently available, (1), (6), to the accuracy of the tables. This gave a ten digit check on the accuracy of this algorithm.

These accuracy tests were made for values of the argument z in the domain

$$|z| \leq 8.0. \qquad (5)$$

IV. The Hypergeometric Function for Values Within the Unit Circle on the Complex Plane.

The hypergeometric function, hereafter termed $F(\alpha, \beta; \gamma; z)$, is the solution to the hypergeometric differential equation. The most compact form of the hypergeometric operator is due to Poole (7) and takes the form:

$$L = z(1-z)\, d^2/dz^2 + [\gamma - (\alpha+\beta+1)z]\, d/dz - \alpha\beta. \tag{1}$$

$F(\alpha, \beta; \gamma; z)$ satisfies the homogeneous relation

$$L\, F(\alpha, \beta; \gamma; z) = 0. \tag{2}$$

The complex plane must be divided into two domains to achieve a viable representation of the hypergeometric function. These two regions are the closed bounded domain

$$|z| \leq 1, \tag{3}$$

and the open infinite domain

$$|z| > 1. \tag{4}$$

The treatment of the hypergeometric function given in this section will pertain only to the unit circle, defined in equation (IV 3). Since L is a second order, linear differential operator, there will be two independent solutions defined by relation (IV 2). The solution to (IV 2) which is generally called the hypergeometric function was first extensively investigated by Gauss (8). Because this function's development was largely dependent on Gauss' work, the function ${}_2F_1(\alpha, \beta; \gamma; z)$

treated here is often called Gauss' series to distinguish it from other solutions to (IV 2).

The second independent solution to (IV 3)can be represented by

$$ {}_2f_1(z) = z^{1-\gamma}\ {}_2F_1(\alpha+1-\gamma, \beta+1-\gamma;\ 2-\gamma;\ z) \quad |\arg z| < \pi,\ |z| \leq 1 \qquad (5) $$

where the principal value branch cut has been used.

The solution to (IV 2) denoted by ${}_2F_1(\alpha,\ \beta;\ \gamma;\ z)$ is a single-valued, analytical function in the domain considered and thus is regular at the origin. Because of its single-valued nature, no branch cut need be defined for this function within the unit circle. Since only hypergeometric series with two numerator parameters and one denominator parameter will be considered, the subscripts, 2 and 1 on the function label will be dropped. The numerator parameters of this function are α and β. The denominator parameter of $F(\alpha, \beta;\ \gamma;\ z)$ is γ.

It should be emphasized that the term "hypergeometric function" is used here to denote that solution to equation (IV 2) which is regular at all points within the unit circle and has been historically labeled Gauss' series. Other dependent or independent solutions of (IV 2), such as the function of ${}_2f_1$ defined in equation (IV 5), are not treated in this discussion.

Mathematical Method

A representation for the hypergeometric function must be developed within the domain of equation (IV 3). For the most general case, $F(\alpha,\ \beta;\ \gamma;\ z)$ will be defined by Gauss' series:

$$ F(\alpha,\ \beta;\ \gamma;\ z) = \sum_{n=0}^{\infty} \alpha_n \beta_n z^n / [\gamma_n n!] \qquad (6) $$

where

$$\alpha_0 = 1 \quad \alpha_n = \alpha*(\alpha+1)*(\alpha+2)*\cdots*(\alpha+n-1) \tag{7}$$

and γ is not a non-positive integer. This series representation is the most functional form for $F(\alpha, \beta; \gamma; z)$ when a programable definition for the function is sought.

The specification that γ is not a non-positive integer is required because definition (IV 6) requires additional restrictions in such a case. There are three cases to consider when any of $\{\alpha, \beta, \gamma\}$ become elements of the set of all non-positive integers, N:

$$N = \{-n \,|\, n = 0, 1, 2, 3, \cdots\}.$$

These cases are:

Case 1: The numerator parameters α and/or β are elements of N.

Case 2: Only the denominator parameter, γ, is an element of N.

Case 3: Parameters of each type, α and/or β, and γ are elements of N.

Special treatment must be given to each of these parameter combinations.

Case 1: When only the numerator parameters, α and/or β, are negative integers or zero, the function defined by (IV 6) becomes a polynomial. This limited power series is a valid representation of F and is used as the hypergeometric function for this case.

Case 2: Whenever γ is an element of N, Gauss' series has a pole. Hence, for all $\gamma = -n$,

$$|F(\alpha, \beta; \gamma; z)| = \infty. \tag{8}$$

Rational functions can be developed which do not possess poles at the non-positive integer values of γ but still satisfy (IV 2). Such

functions are not treated by this algorithm. (see case 2, Section V).

Case 3. In the situation where there are elements of N amongst both the numerator and denominator parameters, the relative magnitudes of the parameters determine if the hypergeometric function converges or has a pole.

Since the hypergeometric function is symmetric in α and β

$$F(\alpha,\ \beta;\ \gamma;\ z) = F(\beta,\ \alpha;\ \gamma;\ z), \tag{9}$$

let α be the numerator parameter that is a negative integer. If both α and β are negative integers, then let α be the parameter value with the smallest magnitude.

$$|\alpha| \leq |\beta|.$$

Case 3a. The numerator parameter has a smaller magnitude than the denominator parameter

$$|\alpha| \leq |\gamma|$$

$$\alpha = -\,m \qquad \gamma = -\,(m+n)$$

$$m = 0,\ 1,\ 2,\ \cdots \qquad n = 0,\ 1,\ 2,\ \cdots$$

For this case, equation (IV 6) still applies but a formula must be defined to avoid ambiguity when $\alpha = \gamma = -\,m$. The definition of $F(\alpha,\ \beta;\ \gamma;\ z)$ is

$$F(-m,\ \beta;\ -(m+n);\ z) = \sum_{r=0}^{m} \frac{(-m)_r (\beta)_r}{(-(m+n))_r\, r!}\, z^r. \tag{10}$$

Case 3b: The numerator parameter has a larger magnitude than the denominator parameter

$$|\alpha| > |\gamma|.$$

In this situation, the hypergeometric function has a pole.

With the special integer cases treated, the hypergeometric function is completely defined within the domain $|z| \leq 1$. The convergence and accuracy of this function will be treated in section V since this algorithm is a special case of $F(\alpha, \beta; \gamma; z)$ on the entire complex plane.

Possible Errors

If the series calculation does not give a relative single term contribution of 1.0×10^{-6} or less after one hundred terms of equation (V 4) have been calculated, the routine prints an error message and terminates the calculation. The value obtained by the one-hundred term sum is returned as the estimate of the function.

If the value of the gamma parameter is a negative integer and meets the specifications of case 2 or case 3b described above, a value of

$$F(\alpha, \beta; -n; z) = 1.0 \times 10^{65} + 1.0 \times 10^{65} i$$

is returned for the function.

V. The Hypergeometric Function on the Complex Plane

When the differential equations of mathematical physics were formulated in differential form in the late 1600's, it was assumed that all problems representing a physical process could be solved with appropriate combinations of elementary functions. The first indication of the need for functions beyond those already known came in 1671 when Newton (9) created a solution to several first order, differential equations by infinite series.

This method provided representation for what later became known as orthogonal polynomials and special functions. The hypergeometric function originated as a real variable series representing a solution to equation (V 2). When special functions were recognized as entities distinct from their series representations, the complete hypergeometric function for the real line and the complex plane was defined.

The creation of $F(\alpha, \beta; \gamma; z)$ for several computational tests has followed this historical development. The function was first needed within the unit circle on the complex plane and its series representation was programed as described in section IV. Later work became dependent on a representation of $F(\alpha, \beta; \gamma; z)$ for the entire complex plane and, therefore, an additional algorithm was developed to evaluate the hypergeometric function in this region.

The formulas presented here represent an analytical continuation of Gauss' series for all z. Other solutions to the hypergeometric differential equation can be prepared by using appropriate linear combinations for the series parameters and multiplying the series value by

an additional function of the independent variable, z.

Mathematical Method

The more expansive form of $F(\alpha, \beta; \gamma; z)$ is more difficult to formulate than the algorithm of $F(\alpha, \beta; \gamma; z)$ within the unit circle. Several methods exist to create Gauss' series for the hypergeometric equation, (IV 2), but the simplest route to the representation of $F(\alpha, \beta; \gamma; z)$ which is useful as an algorithm is by using the integral

$$I = -\frac{1}{2\pi i} \int_P \frac{\Gamma(\alpha+s)\ \Gamma(\beta+s)\ \Gamma(-s)}{\Gamma(\gamma+s)} (-z)^s\, ds \qquad (1)$$

where s is a complex variable and $|\arg(-z)| < \pi$.

Cognizance of the branch cut that has just been defined is very important. This cut must be kept for all complex functions that will be used in the development of the hypergeometric function. The cut is defined on the real axis from 1 to $+\infty$ and is often called the f-cut. The complex plane for the variable z is not defined in normal calculations by this branch cut but rather, takes the form

$$z = re^{i\theta} \qquad -\pi < \theta \leq \pi.$$

Transforming z to the f-cut gives

$$z_T = r\, e^{i\theta} \qquad -2\pi < \theta \leq 0.$$

This rotation of the complex plane about the origin defines all functions involved in $F(\alpha, \beta; \gamma; z)$ with respect to the same cut.

The integral function (V 1) satisfies equation (IV 2) for all z. Thus, it constitutes a solution to the hypergeometric equation

and could be termed a hypergeometric function. Unevaluated, I does not give a programable form to the solution of (IV 2) it represents. The integral I must be evaluated along some contour in the complex plane. The choice of contours in the s plane is dictated by the singularities of the gamma functions contained in I.

For $|z|<1$, the contour for I must contain all singularities of the function $\Gamma(-s)$. These poles will be on the positive real axis so let the contour, P, be any closed curve separating all integers on the positive real axis from the poles of $\Gamma(\alpha+s)$ and $\Gamma(\beta+s)$.

By Cauchy's theorem, the complex integral of a function is the sum of the residues of the function at its poles. The residue of $\Gamma(-s)$ is $(-1)^n/n!$, $s = n$, and thus,

$$I = -1/2\pi i \int_P \frac{\Gamma(\alpha+s)\,\Gamma(\beta+s)\,\Gamma(-s)}{\Gamma(\gamma+s)} (-z)^s\, ds = \sum_{n=0}^{\infty} \frac{\Gamma(\alpha+n)\,\Gamma(\beta+n)}{\Gamma(\gamma+n)n!} z^n,$$

$$|z| < 1. \qquad (2)$$

This relationship implies that I is the regular hypergeometric function for the unit circle of the complex plane. Therefore, the integral I is a representation of the regular solution of (IV 2), and since I is an analytic function of z, it represents $F(\alpha, \beta; \gamma; z)$ for all values of z on the surface $|\arg(-z)| < \pi$.

Solving the integral I for $|z|>1$, will yield a representation of F for the unbounded section of the complex plane. To obtain a solution of I for $|z|>1$, let the contour P enclose all first

order poles of $\Gamma(\alpha+s)$ and $\Gamma(\beta+s)$. The special cases where a contour encloses higher order poles will be treated separately.

Summing the residues of the integral at the poles of $\Gamma(\alpha+s)$ and $\Gamma(\beta+s)$ gives:

$$I = \sum_{n=0}^{\infty} \frac{\Gamma(\beta-\alpha-n)}{\Gamma(\gamma-\alpha-n)} \Gamma(\alpha+n)(-z)^{-\alpha-n}(-1)^n/n! \qquad (3)$$

$$+ \sum_{n=0}^{\infty} \frac{\Gamma(\alpha-\beta-n)}{\Gamma(\gamma-\beta-n)} \Gamma(\beta+n)(-z)^{-\beta-n}(-1)^n/n! \quad |z|>1$$

or

$$F(\alpha,\beta;\gamma;z) = (-z)^{-\alpha} \frac{\Gamma(\beta-\alpha)\Gamma(\gamma)}{\Gamma(\beta)\Gamma(\gamma-\alpha)} \sum_{r=0}^{\infty} \frac{(\alpha)_r(1-\gamma+\alpha)_r}{(1-\beta+\alpha)_r r!\, Z^r} \qquad (4)$$

$$+ (-z)^{-\beta} \frac{\Gamma(\gamma)\Gamma(\alpha-\beta)}{\Gamma(\alpha)\Gamma(\gamma-\beta)} \sum_{r=0}^{\infty} \frac{(\beta)_r(1+\beta-\gamma)_r}{(1+\beta-\alpha)_r r!\, Z^r} \quad |z|>1.$$

Thus, the extension of the hypergeometric function to the entire complex plane is virtually complete. A discussion of the convergence of I and the exact distribution of all contours is contained in (10).

The definition of equation (V4) holds for most values of the parameters α, β, γ. Unfortunately, the difficulty of representing F outside the unit circle predominately centers on the significant number of special cases that arise for specific values of γ, α or β. Each of these specific situations will be treated in turn and the formulas that result will be detailed. In all of the discussion that follows, the domain of the independent variable, z, will be $|z| > 1$.

Case 1: At least one of the numerator parameters, α or β, is a non-

positive integer.

For this situation, the series presented in equation (IV 6) terminates after $|\alpha| + 1$ or $|\beta| + 1$ terms. This formula enters the analytical continuation of the function at this point because of the pole pattern of the integral, I.

When the contour, P, for the evaluation of I is drawn, it is designed to isolate poles of $\Gamma(\alpha+s)$, $\Gamma(\beta+s)$ and $\Gamma(-s)$. However, if α or $\beta = -n$, then some poles coincide and a series of higher order poles appear on the f-cut. The summation of these residue terms shows that formula (IV 6) covers this special coincidence of poles.

For $\alpha = -n$, $|z| > 1$ and $|\arg(-z)| < \pi$,

$$F(-n, \beta; \gamma; z) = \sum_{i=0}^{n} \frac{(-n)_i(\beta)_i}{i!(\gamma)_i} z^i. \qquad (5)$$

Since F is symmetric in its numerator parameters, no separate definition is needed for $\beta = -n$.

Case 2. The denominator parameter, γ, is a non-positive integer.

The single analytic function $F(\alpha, \beta; \gamma; z)$ defined by the f-cut on the z plane, has poles at all negative integer values of γ. Thus, F is a meromorphic* function of γ. Because of this behavior, the standard function $F(\alpha, \beta; \gamma; z)$ defined from integral (V 2) obeys the condition

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* A function of the complex variable z is said to be meromorphic in a domain D if it is analytic in D except for a finite number of poles. P231, Mathematics Dictionary, Editors: G. James and R. C. James, Van Nostrand, (1949).

$$|F(\alpha, \beta; -n; z)| = \infty \quad n = 0, 1, 2, \ldots \tag{6}$$

$\forall\ \alpha, \beta$ not covered in the following cases and $\forall$ z. The algorithm meets the conditions of this case by returning a very large, first quadrant, complex number as the value of $F(\alpha, \beta; \gamma; z)$.

There exist certain parameter combinations which allow γ to be a non-positive integer while Gauss' series remains finite. These situations will be considered in the cases which follow.

An important formula associated with the parameter combination of case 2 should be mentioned. This relationship is the definition of the hypergeometric function in terms of a quotient function, $Q(\alpha, \beta; \gamma; z)$. The definition of Q is

$$Q(\alpha, \beta; \gamma; z) = F(\alpha, \beta; \gamma; z)/\Gamma(\gamma). \tag{7}$$

The combination of functions, $F(\alpha, \beta; \gamma; z)/\Gamma(\gamma)$, is an analytic function of all of its parameters for all of their values and it has been used by several authors (11) to define a finite value for the hypergeometric function at the parameter values $\gamma = -n$, $n = 0, 1, 2, \ldots$ It must be emphasized that these efforts to remove the poles of $F(\alpha, \beta; \gamma; z)$ on the γ plane are valid only within a loose definition of the term "hypergeometric function."

Using this label to denote any function which satisfies the hypergeometric equation (IV 2), allows $Q(\alpha, \beta; \gamma; z)$ to be termed a hypergeometric function. Gauss' series can then be used as the definition of a solution to (IV 2) but the limit of $Q(\alpha, \beta; \gamma; z)$ can be inserted in such a definition when $\gamma = -n$. The value of Q in this case (12) is

$$\lim_{\gamma \to -n} Q(\alpha,\ \beta\ ;\ \gamma;\ z) = \frac{(\alpha)_{n+1}(\beta)_{n+1}}{(n+1)!}\ z^{n+1}\ F(\alpha+n+1,\ \beta+n+1;\ n+2;\ z) \quad (8)$$

See equation (IV 7) concerning the notation $(\alpha)_{n+1}$.

The hypergeometric function programmed for the algorithm defined here is Gauss' series as derived for all cases from integral I of equation (V 2). Values of the quotient function Q, at the appropriate values of γ can be obtained by the use of this algorithm and the right hand side of equation (V 8).

Case 3. The difference $\alpha-\beta$ is an integer.

It was noted previously that equation (V 4) only applied when the poles contained in the contour were first order. When $|\alpha-\beta| = n$, this limit is broken and the representation of $F(\alpha,\ \beta;\ \gamma;\ z)$ must be recalculated. This failure of (V 4) is apparent in the structure of the equation itself. The multipliers $\Gamma(\alpha-\beta)$ or $\Gamma(\beta-\alpha)$ possess poles at the non-positive integer values of their argument. Hence, whenever $\alpha-\beta$ is equal to an integer, at least one of these multipliers is infinite.

The alterations to derive a formula for this case must start with the contour for integrating I in equation (V 2). The contour is normally set up to envelop the poles of $\Gamma(-s)$ or those of $\Gamma(\alpha+s)$ and $\Gamma(\beta+s)$. Each of these three sets of poles is assumed separate and distinct. When $\alpha-\beta$ is an integer, some of the poles of $\Gamma(\alpha+s)$ and $\Gamma(\beta+s)$ coincide. Since the poles are

$$s = -(m+\alpha) \quad \text{and} \quad s = -(m'+\beta),$$

then

$$\alpha - \beta = n,$$

gives

$$s = -m - (n + \beta) \qquad s = -m' - \beta, \tag{9}$$

where

$$m,\ m',\ n = 0,\ 1,\ 2,\ \ldots$$

For some values of s, both elements of equation (V 9) will be satisfied simultaneously and this point will constitute a second order pole of I. Thus the residue of I changes at these s values and correspondingly, the formula for $F(\alpha, \beta; \gamma; z)$ changes. If I is integrated along a contour containing all poles of equation (V 9), the altered sum of all residues gives the representation

$$F(\alpha,\ \alpha+n;\ \gamma;\ z) = \Gamma(\gamma)/[\,\Gamma(\alpha+n)(-z)^{\alpha}]\ \{\ \sum_{r=0}^{n-1} \frac{(\alpha)_r^{*}\ \Gamma(n-r)}{\Gamma(\gamma-\alpha-r)r!}\ z^{-r} \tag{10}$$

$$+\ 1/[\,\Gamma(\gamma-\alpha)(-z)^{n}]\ \sum_{r=0}^{\infty} \frac{(\alpha)_{n+r}(1-\gamma+\alpha)_{n+r}}{r!\ \ (n+r)!}\ z^{-r}\ [\mathrm{Log}_e(-z) + \mathrm{Psi}(r)]\}$$

where $\mathrm{Psi}(r) = \psi(1+n+r) + \psi(1+r) - \psi(\alpha+r+n) - \psi(\gamma-\alpha-r-n)$. An alternative formula for this case is derived in Appendix A.

This formula must be used to evaluate $F(\alpha,\ \beta;\ \gamma;\ z)$ when $\alpha-\beta=n$, $|z| > 1$, unless $\gamma - \alpha$ is also an integer. This parameter pattern is treated in case 4.

Case 4. The parameter difference $\alpha - \beta$ and $\gamma - \alpha$ are both integer.

The behavior of $F(\alpha,\ \beta;\ \gamma;\ z)$ in this case is determined by the sign of the integer difference $\gamma - \alpha$. Let $|\alpha-\beta| = n$ and $\gamma - \alpha = -m$, $n = 0,\ 1,\ 2,\ \cdots;\ m = 1,\ 2,\ 3,\ \cdots$

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* If $n = 0$, $n - 1 = -1$, then this sum is zero.

In this situation, the negative integer difference of $\gamma-\alpha$ allows the use of an elementary transform on $F(\alpha, \beta; \gamma; z)$ which creates a polynomial form for the function. This result is detailed in case 5.

$$\text{Let } |\alpha - \beta| = n \text{ and } \gamma - \alpha = m. \quad n, m = 0, 1, 2, \ldots$$

An exception to case 3 exists only if $m = n + \ell$ where $\ell = 0, 1, 2, \ldots$ The term α has been taken to have the smaller magnitude of the two numerator parameters. When these criteria are met, the function of the contour integral I simultaneously has three poles. This situation must be covered by a limiting process on equation (V 10). The result (13) is

$$\lim_{\gamma \to \alpha+n+\ell} F(\alpha, \alpha+n; \gamma; z) = \tag{11}$$

$$\Gamma(\alpha+n+\ell) / [(-z)^{\alpha}\, \Gamma(\alpha+n)] \{(-1)^{n+\ell}(-z)^{-n} \sum_{r=\ell}^{\infty} \frac{(\alpha)_{r+n}(r-\ell)!}{(n+r)!\,r!} z^{-r}$$

$$+ \frac{(-z)^{-n}}{(\ell+n-1)!} \sum_{r=0}^{\ell-1} \frac{(\alpha)_{r+n}(1-n-\ell)_{r+n}}{r!\,(r+n)!} z^{-r} [\mathrm{Log}_e(-z)+\mathrm{Pzi}(r)]^{*}$$

$$+ \sum_{r=0}^{n-1} \frac{(n-r-1)!\,(\alpha)_r}{(n+\ell-r-1)!\,r!} z^{-r}\}^{**},$$

$$\mathrm{Pzi}(r) = \psi(1+n+r) + \psi(1+r) - \psi(\alpha+n+r) - \psi(\ell-r).$$

If $m > 0$ but $m < n$, then the formula of case 3 applies.

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* If $\ell = 0$, $\ell - 1 = -1$, then this sum is zero.

**If $m = 0$, $m - 1 = -1$, then this sum is zero.

Case 5. One or both of the parameter differences $\gamma - \alpha$ or $\gamma - \beta$ is a negative integer.

This occurence has already been alluded to under case 4. Whenever one of the two parameter differences, $\gamma - \alpha$ or $\gamma - \beta$ is a negative integer, an Euler transform of the hypergeometric function can be completed. This transform creates a terminating polynomial representation for $F(\alpha, \beta; \gamma; z)$. In general, this transform only holds when $|z| < 1$ or the parameters meet the conditions of this case.

The result of the transform is

$$\gamma - \alpha = -n \text{ or } \gamma - \beta = -n' \qquad n, n' = 1, 2, 3, \ldots$$

$$F(\alpha, \beta; \gamma; z) = (1-z)^{\gamma-\alpha-\beta} F(\gamma-\alpha, \gamma-\beta; \gamma; z). \tag{12}$$

Should it occur that $\gamma = -n$ and α or $\beta = n'$, then

$$\gamma - \alpha = -(n + n').$$

However, this situation is still considered to represent a negative integer value for γ and nothing more. Hence, the equations of case 2 apply and

$$|F(n', \beta; -n; z)| = \infty \tag{13}$$

The definition of the hypergeometric function is complete. The complete list of all components of the algorithm for calculating $F(\alpha, \beta; \gamma; z)$ is presented in Table 2.

Tests of the Algorithm within the Unit Circle

The function $F(\alpha, \beta; \gamma; z)$ reduces to well known transcendental

functions for specific choices of the parameters α, β and γ if z is an element of the domain $|z| < 1$. The equations resulting from this reduction in form were used as tests of the validity of the algorithm discussed in section IV.

The equations (14) used in verifying this algorithm were:

$$z\ F(\tfrac{1}{2},\ \tfrac{1}{2};\ \tfrac{3}{2};\ z^2) = \text{arc sin}\ (z) \tag{14}$$

$$z\ F(1,\ 1;\ 2;\ z) = -\text{Log}_e(1 - z) \tag{15}$$

$$2\ F(-w/2, (1-w)/2;\tfrac{1}{2};\ z^2) = (1+z)^w + (1-z)^w \tag{16}$$

$|z| < 1$, w unrestricted (it may be complex).

Tests of the Algorithm for the Full Complex Plane

The flexibility of the hypergeometric function makes it a difficult function to test. Few relationships of the function have sufficient flexibility to cover all of its variations but a test was sought which would hold in almost all cases.

The class of equalities termed quadratic transforms of $F(\alpha, \beta; \gamma; z)$ yielded a testing equation for the algorithm. A quadratic transform of Gauss' series is a substitution of a second order polynomial for the independent variable z, which establishes an equality between the two resulting functions. A compact but lucid discussion of the criteria governing the existence of a quadratic transform and a compendium of quadratic transforms will be found in Oberhettinger and Magnus (15).

The quadratic transform used for all tests beyond the unit circle was

$$w = [\sqrt{1-z} - 1]/[\sqrt{1-z} + 1]. \qquad (17)$$

The utility of this mapping is shown in Figures 1 and 2. This relationship maps all of the z plane into the unit circle on the complex w plane. Within $|w| < 1$, the value of Gauss' series can be checked through the relations defined previously. The equation of the transform (16) for a given set of parameters and a set value of the variable z, is:

$$F(\alpha, \beta; \alpha+\beta+\tfrac{1}{2}; z) = \left(\frac{1+\sqrt{1-z}}{2}\right)^{-2\alpha} F\left(2\alpha, \alpha-\beta+\tfrac{1}{2}, \alpha+\beta+\tfrac{1}{2}, \frac{\sqrt{1-z}-1}{\sqrt{1-z}+1}\right). \qquad (18)$$

By judicious choice of the two parameters, α and β, all variations in α, β, γ and z could be checked. Approximately one thousand tests of the routine were made.

Further Points on Quadratic Transforms

Several different quadratic transforms were tried as tests for the hypergeometric function subroutine. All of these transforms were based on the variable relationship of equation (V 17). Two transforms

$$F(2\alpha, 2\alpha+1-\gamma; \gamma; w) = (1-w)^{-2\alpha} F(\alpha, \gamma-\alpha+\tfrac{1}{2}; \gamma; -4w/(w-1)^2) \qquad (19a)$$

and

$$F(\alpha, \gamma-\alpha+\tfrac{1}{2}; \gamma; z) = \left(\frac{1+\sqrt{1-z}}{2}\right)^{-2\alpha} F\left(2\alpha, 2\alpha+1-\gamma; \gamma; \frac{\sqrt{1-z}-1}{\sqrt{1-z}+1}\right). \qquad (19b)$$

contained in a major work in the literature on hypergeometric functions (17) were found to be wrong.

The error is introduced into these equations when the use of an Euler transform necessitates creating the difference a-b where

$$a = \gamma \qquad b = \alpha + \tfrac{1}{2}.$$

The result is listed as

$$a - b = \gamma - \alpha + \tfrac{1}{2},$$

rather than the correct form

$$a - b = \gamma - \alpha - \tfrac{1}{2}.$$

The correct transforms are

$$F(2\alpha,\ 2\alpha+1-\gamma;\ \gamma;\ w) = (1-w)^{-2\alpha}\, F(\alpha,\ \gamma-\alpha-\tfrac{1}{2};\ \gamma;\ -4w/(w-1)^2) \qquad (20a)$$

and

$$F(\alpha,\ \gamma-\alpha-\tfrac{1}{2};\ \gamma;\ z) = \left(\frac{1+\sqrt{1-z}}{2}\right)^{-2\alpha} F\left(2\alpha,\ 2\alpha+1-\gamma;\ \gamma;\ \frac{\sqrt{1-z}-1}{\sqrt{1-z}+1}\right), \qquad (20b)$$

valid for all z.

Accuracy of the Function

The algorithm prepared to calculate $F(\alpha, \beta; \gamma; z)$ creates the value of the function at any point within a mean relative error of 10^{-6} units, when single precision arithmetic is used. The double precision routine contains an accuracy test for a mean relative error of 10^{-11} units. When this level of accuracy can not be achieved, the subprogram prints an error message and returns the best approximation to the functions' value that would be achieved with one hundred terms of the appropriate series.

Convergence of the Algorithm

The series representations derived from integral (V 1) can be shown to be absolutely convergent for all values of z save $|z| = 1$. In this numerical application where the hypergeometric function is represented by a finite series, all representations have been found to converge within a fixed tolerance for all values of z save those within a certain distance on either side of the unit circle, $|z| \leq 1$.

This region of divergence can be represented by

$$|z_d| = 1 \pm \epsilon(\alpha, \beta, \gamma). \tag{21}$$

As indicated by equation (V21), the region on the z plane in which $F(\alpha, \beta; \gamma; z)$ will be found to diverge is a function of the parameters, α, β, and γ.

In general, $\epsilon(\alpha, \beta, \gamma)$ is quite small and ordinarily is less than one tenth of a unit.

$$|\epsilon(\alpha, \beta, \gamma)| \leq 0.1. \tag{22}$$

However, as the number Real $(\gamma-\alpha-\beta)$ becomes more negative, $\epsilon(\alpha, \beta, \gamma)$ can exceed the bounds of equation (V22). The only definite rule that defines the region of divergence of this algorithm once Real $(\gamma-\alpha-\beta)$ has become less than -1 is that the more negative Real $(\gamma-\alpha-\beta)$ becomes, the greater the area of divergence in the z plane becomes.

Table 1

Values of the Bernoulli Numbers, β_n, to 15 Digits

n	β_n	n	β_n
2	$1.66666666666667 \times 10^{-1}$	28	$2.72982310678161 \times 10^{7}$
4	$-3.33333333333333 \times 10^{-2}$	30	$6.01580873900642 \times 10^{8}$
6	$2.38095238095238 \times 10^{-2}$	32	$-1.51163157670922 \times 10^{10}$
8	$-3.33333333333333 \times 10^{-2}$	34	$4.29614643061167 \times 10^{11}$
10	$7.57575757575758 \times 10^{-2}$	36	$-1.37116552050883 \times 10^{13}$
12	$2.53113553113553 \times 10^{-1}$	38	$4.88332318973593 \times 10^{14}$
14	1.66666666666666	40	$-1.92965793419401 \times 10^{16}$
16	7.09215686274510		
18	$5.49711779448622 \times 10^{1}$	42	$8.41693047573682 \times 10^{17}$
		44	$-4.03380718540594 \times 10^{19}$
20	$-5.29124242424242 \times 10^{2}$	46	$2.11507486380820 \times 10^{21}$
22	$6.19212318840580 \times 10^{3}$	48	$-1.20866265222965 \times 10^{23}$
24	$-8.65802531135531 \times 10^{4}$	50	$7.50086674607696 \times 10^{24}$
26	$1.42551716666667 \times 10^{6}$	52	$-5.03877810148107 \times 10^{26}$

Table 2

Hypergeometric Function Formulas

Domain	Special Case				Formula for $F(\alpha, \beta; \gamma; z)$
	α	β	γ		
1) all z	not a non-positive integer	not a non-positive integer	-n		$F(\alpha, \beta, -n, z) = \pm\infty$
2) all z	negative integer -m and/or	negative integer -m	-n	$-n=-m, -(m+1), \ldots$ $\lvert n\rvert \geq \lvert m\rvert$	$F(\alpha, \beta; \gamma; z) = \sum_{r=0}^{m} \frac{(-m)_r(\beta)_r}{(-n)_r\, r!} z^r$
3) $\lvert z\rvert<1$	all values not covered by 1) or 2)	all values not covered by 1) or 2)	all values not covered by 1) or 2)		$F(\alpha, \beta; \gamma; z) = \sum_{r=0}^{\infty} \frac{(\alpha)_r(\beta)_r}{(\gamma)_r\, r!} z^r$
4) $\lvert z\rvert>1$	-n and/or	-n	not a non-positive integer		$F(\alpha,\beta; \gamma; z) = \sum_{r=0}^{n} \frac{(\alpha)_r(\beta)_r}{(\gamma)_r\, r!} z^r$
5) $\lvert z\rvert>1$	not a non-positive integer	not a non-positive integer	number not satisfying cases, 1), 6), 7)	$\lvert\alpha - \beta\rvert = n$	$F(\alpha, \beta; \gamma; z) = \Gamma(\gamma)/(\Gamma(\alpha+n)(-z)^{\alpha})*$ $\{\sum_{r=0}^{n-1} \frac{(\alpha)_r\Gamma(n-r)}{\Gamma(\gamma-\alpha-r)r!} z^{-r} + [\Gamma(\gamma-\alpha)(-z)^n]^{-1} \sum_{r=0}^{\infty} \frac{(\alpha)_{n+r}(1-\gamma+\alpha)_{n+r}}{r!(n+r)!} z^{-r}*$ $[\mathrm{Log}_e(-z) + \psi(1+n+r) + \psi(1+r) - \psi(\alpha+r+n) - \psi(\gamma-\alpha-r-n)]$
6) $\lvert z\rvert>1$	not a non-positive integer	not a non-positive integer	value such that $\gamma-\alpha=\lvert\alpha-\beta\rvert+m$	$\lvert\alpha - \beta\rvert = n$	$F(\alpha, \alpha+n; \alpha+n+m; z) = \frac{\Gamma(\alpha+n+m)}{(-z)^{\alpha}\Gamma(\alpha+m)} *$ $\{(-1)^{m+n}(-z)^{-n} \sum_{r=m}^{\infty} \frac{(\alpha)_{r+n}(r-m)!}{(n+r)!\, r!} z^{-r}$ $+\frac{(-z)^{-n}}{(m+n-1)!} \sum_{r=0}^{m-1} \frac{(\alpha)_{r+n}(1-n-m)_{r+n}}{r!\,(r+n)!} z^{-r}[\mathrm{Log}_e(-z) + \mathrm{Pzi}(r)]$ $+ (-z)^{-\alpha} \sum_{r=0}^{n-1} \frac{(n-r-1)!\,(\alpha)_r}{(n+m-r-1)!\,r!} z^{-r}\}$ $\mathrm{Pzi}(r) = \psi(1+n+r) + \psi(1+r) - \psi(\alpha+n+r) - \psi(m-r)$

Table 2 (continued)

Domain		Special Case α	Special Case β	Special Case γ	Formula for $F(\alpha, \beta; \gamma; z)$
7)	$\lvert z\rvert > 1$	not a non-positive integer	not a non-positive integer	value such that $\gamma-\alpha=-n$ and $\gamma-\beta=-m$	$F(\alpha,\beta;\gamma;z) = (1-z)^{\gamma-\alpha-\beta} F(\gamma-\alpha, \gamma-\beta; \gamma; z)$
8)	$\lvert z\rvert > 1$	all values not covered by the above	all values not covered by the above	all values not covered by the above	$F(\alpha,\beta;\gamma;z) = (-z)^{-\alpha} \frac{\Gamma(\beta-\alpha)\Gamma(\gamma)}{\Gamma(\beta)\Gamma(\gamma-\alpha)} F(\alpha, 1-\gamma+\alpha; 1-\beta+\alpha; 1/z)$ $+(-z)^{-\beta} \frac{\Gamma(\gamma)\Gamma(\alpha-\beta)}{\Gamma(\alpha)\Gamma(\gamma-\beta)} F(\beta, 1+\beta-\gamma; 1+\beta-\alpha, 1/z)$

Figure Captions

1. The z plane with a f cut.

2. The w plane showing the mapping $w = (\sqrt{1-z}-1)/(\sqrt{1-z}+1)$. Corresponding points in the two planes are indicated by the lettering.

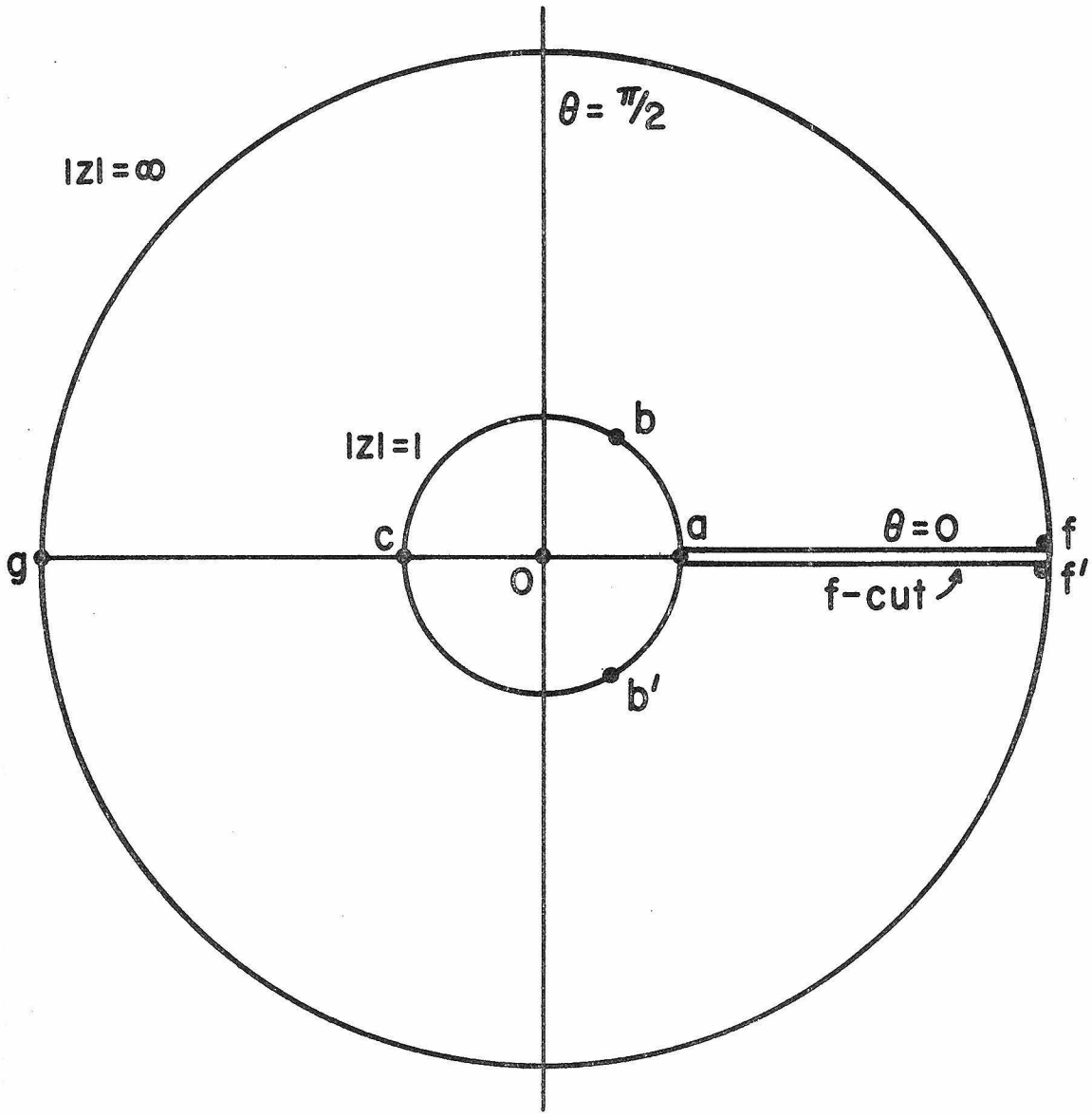

Figure 1

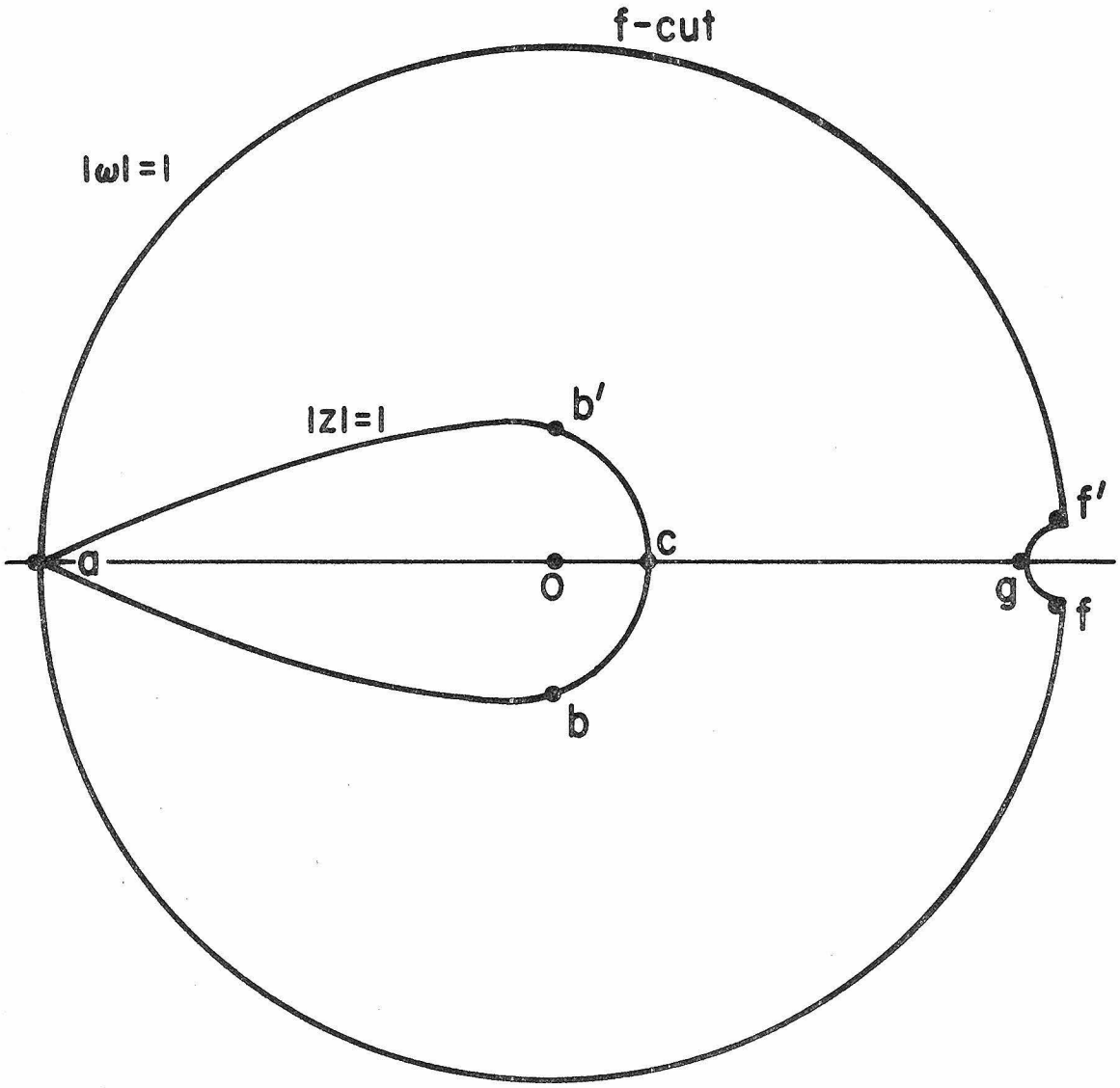

Figure 2

References

1. DAVIS, H. T., Tables of the Higher Mathematical Functions, Volumes 1 and 2, Principia Press, 1933-1935.

2. ABRAMOWITZ, M. and STEGUN, I., Handbook of Mathematical Functions, p. 256, National Bureau of Standards, Applied Mathematics Series, Vol. 55, (1964).

3. ERDELYI, A., MAGNUS, W., OBERHETTINGER, G., and TRICOMI, F. G., Higher Transcendental Functions, Chapter 1, Vol. I, McGraw-Hill, (1953).

4. ABRAMOWITZ, M., and STEGUN, I., Handbook of Mathematical Functions, pp. 257, 6.1.40, National Bureau of Standards, Applied Mathematics Series, Vol. 55, (1964).

5. ABRAMOWITZ, M., and STEGUN, I., Handbook of Mathematical Functions, pp. 804-810, National Bureau of Standards, Applied Mathematics Series, Vol. 55, (1964).

6. ABRAMOWITZ, M., and STEGUN, I., Handbook of Mathematical Functions, pp. 267-273, p. 288, National Bureau of Standards, Applied Mathematics Series, Vol. 55 (1964).

7. POOLE, E. G. C., Introduction to the Theory of Linear Differential Equations, Oxford, (1936).

8. GAUSS, ., GOTTINGER, C., Commentationes Recentiores (1812) T. II; Ges. Werks, T. III, pp. 123-163.

9. Methodus Fluxiorum et Serierum Infinitarum, Issac Newton, Published 1736 but probably composed about 1671.

10. BAILEY, W. R., Generalized Hypergeometric Series, Section 1.6, Cambridge Press, (1935).

11. ERDELYI, A. MAGNUS, W. OBERHETTINGER, F., and TRICOMI, F. G., Higher Transcendental Functions, p. 56, Vol. I, McGraw-Hill, (1953).

12. ABRAMOWITZ, M., and STEGUN, I., Handbook of Mathematical Functions, p. 556, 15.1.2, National Bureau of Standards, Applied Mathematics Series, Vol. 55 (1964).

13. ERDELYI, A. MAGNUS, W., OBERHETTINGER, F., and TRICOMI, E. G., Higher Transcendental Functions, p. 64, Vol. I, McGraw-Hill, (1953).

14. SNOW, C., Hypergeometric and Legendre Functions with Applications to Potential Theory, p. 2, Equations (6a), (6g), (6i), National Bureau of Standards, Applied Mathematics Series, Vol. 19, (1952)

15. MAGNUS, W., OBERHETTINGER, F., SONI, R. P., p. 49, Formulas and Theorems for the Special Functions of Mathematical Physics, Springer Verlag, New York, (1966).

16. SNOW, C., Hypergeometric and Legendre Functions with Applications to Potential Theory, p. 17, (8a), National Bureau of Standards Applied Mathematics Series, Vol. 19, (1952).

17. SNOW, C., Hypergeometric and Legendre Functions with Applications to Potential Theory, pp. 18-19, equations (11a) and (11b), National Bureau of Standards, Applied Mathematics Series, Vol. 19 (1952).

18. BARNES, E. W. Proc. London Math. Soc., (2), 6, 141 (1908).

19. CHURCHILL, R. V., Complex Variables and Applications, Section 58, p. 134, McGraw-Hill (1960).

20. ABRAMOWITZ, M., and STEGUN, I., Handbook of Mathematical Functions, p. 260, 6.5 National Bureau of Standards, Applied Mathematics Series, Vol. 55 (1964).

21. International Business Machines Corporation, System/360, Scientific Subroutine Package, pp. 81-82, Version III, Programer's Manual, GH20-0205-4, (1970).

Appendix A. Alternative Representation for $F(\alpha, \beta; \gamma; z)$ when $|\alpha-\beta| = n$ and $|z|>1$.

The Barnes (18) integral

$$I = \frac{-1}{2\pi i} \int_c \frac{\Gamma(\alpha+s)\Gamma(\beta+s)\Gamma(-s)}{\Gamma(\gamma+s)} (-z)^s \, ds \qquad (1)$$

is a convergent form of the regular hypergeometric function $F(\alpha, \beta; \gamma; z)$ for an appropriate infinite contour, c . Consider the evaluation of I in the case $|\alpha-\beta| = n$ for $|z|> 1$.

Under these conditions, two infinite sets of poles coalesce. The poles are:

for	$\Gamma(\alpha+s)$	$s = -(\ell+\alpha)$	$\ell = 0, 1, 2, \ldots$
for	$\Gamma(\beta+s)$	$s = -(m+\beta)$	$m = 0, 1, 2, \ldots$

Since $|\alpha-\beta| = n$, where α will be assumed to have the smaller magnitude,

$$\beta = \alpha+n \text{ implies } \quad s = -(\ell+\alpha)$$
$$s = -(m+n+\alpha)$$

are both poles of I. Thus, when $\ell = m+n$, s is a pole of both gamma functions and I has a second order pole.

Choose the contour c, such that all poles of $\Gamma(-s)$, the positive integers, lie to the right of the contour and all poles of $\Gamma(\alpha+s)$ and $\Gamma(\beta+s)$ lie to the left of c. This places the basic line of c along the imaginary axis. Complete c so that it encloses all of the left hand poles.

The integral I can be evaluated along c by summing the residues of I at all poles within c. For all points of s such that

$$s = - (\ell+\alpha)$$

but $\ell < n$, the integral I will possess a first order pole. There will be n such poles from $\ell = 0$ to $\ell = n - 1$ and their summed residues are

$$\frac{1}{2\pi i} \sum_{\ell=0}^{n-1} \frac{\Gamma(\beta+s)\Gamma(-s)}{\Gamma(\gamma+s)} (-z)^s \frac{(-1)^\ell}{\ell!} \Bigg|_{s = -(\ell+\alpha)} \tag{2}$$

Inserting the value of s at each pole gives

$$\frac{-(z)^{-\alpha}}{2\pi i} \sum_{\ell=0}^{n-1} \frac{\Gamma(\ell+\alpha)\Gamma(n-\ell)}{\ell!\ \Gamma(\gamma-\ell-\alpha)} (z)^{-\ell}.$$

The second order poles will be evaluated next. Since the combined function $\Gamma(\alpha+s)\Gamma(\beta+s)$ has a second order pole when $s = -(n+\ell+\alpha)$, for all ℓ, the residue of this product function at each such point must be calculated.

This can be accomplished by use of the integral form of the Γ function. The representation is

$$\Gamma(z) = \int_0^\infty e^{-\tau} \tau^{z-1}\, d\tau. \tag{3}$$

The pole in the integral of equation (A 3) occurs at $\tau = 0$. Separate the integral into two terms

$$\begin{aligned} \Gamma(z) &= P(z) + Q(z) \qquad (4) \\ &= \int_0^1 e^{-\tau}\, \tau^{z-1}\, d\tau + \int_1^\infty e^{-\tau}\, \tau^{z-1}\, d\tau. \end{aligned}$$

The term P(z) contains the pole of $\Gamma(z)$ when $z = -m$, $m = 0.1.2...$ Let the two gamma functions of $\Gamma(\alpha+s)\Gamma(\beta+s)$ be represented in this form to give

$$\Gamma(\alpha+s)\Gamma(\beta+s) = (P(\alpha+s) + Q(\alpha+s))(P(\beta+s) + Q(\beta+s)) = \quad (5)$$

$$P(\alpha+s)\ P(\beta+s) + Q(\alpha+s)\ P(\beta+s) + P(\alpha+s)\ Q(\beta+s) + Q(\alpha+s)\ Q(\beta+s).$$

when $s = -(n+\ell+\alpha)$, the first three terms of the right hand side of equation (A 5) possess poles. The residues at these poles can be calculated by use of a Laurent series.

As an example of this process, consider the term $P(\alpha+s)\ Q(\beta+s)$.

$$P(\alpha+s)\ Q(\beta+s) = Q(\beta+s) \int_0^1 e^{-\tau}\ \tau^{\alpha+s-1}\ d\tau. \qquad (6)$$

Expand the function $e^{-\tau}$ in its Maclaurin series,

$$e^{-\tau} = \sum_{j=0}^{\infty} \frac{(-\tau)^j}{j!}$$

and insert this expansion in equation (A 6). This gives

$$Q(\beta+s) \sum_{j=0}^{\infty} \frac{(-1)^j}{j!} \int_0^1 \tau^{j+\alpha+s-1}\ d\tau. \qquad (7)$$

Then, by evaluating the integral on τ,

$$P(\alpha+\beta)\ Q(\beta+s) = Q(\beta+s) \sum_{j=0}^{\infty} \frac{(-1)^j}{j!} \frac{1}{j+\alpha+s}. \qquad (8)$$

Since $s = -(n+\ell+\alpha)$, when $j = n+\ell$, one term of equation (8) has a zero as its denominator. Hence, the residue at $s = -(n+\ell+\alpha)$ of $P(\alpha+s)\,Q(\beta+s)$ is the coefficients of this pole term, which is

$$R = Q(\beta+s)\,(-1)^{n+\ell}/(\ell+n)! \tag{9}$$

For an analysis of the calculation of residues by Laurent series, see (19).

As was mentioned previously, equation (A 5) has three terms which have poles when $s = -(n+\ell+\alpha)$. R represents the residue of only one of those three contributions. The series technique must be repeated for $P(\alpha+s)\,P(\beta+s)$ and $P(\beta+s)\,Q(\alpha+s)$ to obtain the total residue of $\Gamma(\alpha+s)\,\Gamma(\beta+s)$ at the pole point $s = -(n+\ell+\alpha)$.

However, there are an infinite number of such pole points corresponding to the infinite number of values of ℓ, $\ell = 0, 1, 2, \ldots$ Summing all total residues for all possible values of ℓ yields the second order pole contribution to the value of the integral I.

$$I = \frac{1}{2\pi i}\left\{(-z)^{-\beta}\sum_{r=0}^{\infty}\frac{\Gamma(\beta+r)(z)^{-r}}{\Gamma(\gamma-\beta-r)} * \right.$$

$$\left.\left[\left(Q(-r) + \sum_{\ell=0}^{\infty}{}' \frac{(-1)^{\ell}}{\ell!}\,\frac{1}{\ell-r}\right)\frac{(-1)^{n}}{(n+r)!} + \left(Q(-r-n) + \sum_{j=0}^{\infty}{}' \frac{(-1)^{j}}{j!}\,\frac{1}{j-r-n}\right)/r!\right]\right\} \tag{10}$$

$'$ means $\ell \neq r$; $'$ means $j \neq n+r$

These two components combine to give the final form for the hypergeometric function:

$$F(\alpha,\ \beta;\ \gamma;\ z) = \left[\frac{\Gamma(\gamma)}{\Gamma(\alpha)\,\Gamma(\beta)}\right]\left\{(-z)^{-\alpha}\sum_{\ell=0}^{n-1}\frac{\Gamma(\ell+\alpha)\,\Gamma(n-\ell)}{\ell!\ \Gamma(\gamma-\ell-\alpha)}\,(z)^{-\ell}\right. \tag{11}$$

$$\left. + (-z)^{-\beta}\sum_{\ell=0}^{\infty}\frac{\Gamma(\beta+\ell)(z)^{-\ell}}{\Gamma(\gamma-\beta-\ell)} * \right.$$

$$\left[\left(Q(-r) + \sum_{m=0}^{\infty}{}' \frac{(-1)^m}{m!}\frac{1}{m-\ell}\right)\frac{(-1)^n}{(n+\ell)!} + \left(Q(-\ell-n) + \sum_{j=0}^{\infty}{}' \frac{(-1)^j}{j!}\frac{1}{j-\ell-n}\right)/\ell!\right]\right\}.$$

$'$ means $m \neq \ell$ $\qquad$ $'$ means $j \neq n+\ell$

The function $Q(z)$ is the incomplete gamma function (21)

$$Q(z) = \Gamma(z,\ 1) = \int_1^{\infty} e^{-\tau}\ \tau^{z-1}\ d\tau.$$

This function can be evaluated by several standard mathematical techniques (21).

Algorithm 1a

Single Precision Exponentiation Function

```
      COMPLEX FUNCTION COMPOW(X,Y)                                          CMPW  10
C THIS ROUTINE COMPUTES THE RESULT OF RAISING THE COMPLEX VARIABLE X TO CMPW  20
C THE COMPLEX POWER Y. IF X AND Y HAVE ZERO IMAGINARY PARTS, THEN IT    CMPW  30
C COMPUTES THE VALUE OF X RAISED TO AN ARBITRARY REAL POWER.            CMPW  40
      COMPLEX X,Y,CEXP,CLOG                                             CMPW  50
      IF(CABS(X)) 1,1,3                                                 CMPW  60
    3 COMPOW=CEXP(Y*CLOG(X))                                            CMPW  70
      RETURN                                                            CMPW  80
    1 IF(CABS(Y)) 2,2,4                                                 CMPW  90
    2 COMPOW=(1.0,0.0)                                                  CMPW 100
      RETURN                                                            CMPW 110
    4 COMPOW=(0.0,0.0)                                                  CMPW 120
      RETURN                                                            CMPW 130
      END                                                               CMPW 140
```

Algorithm 1b

Double Precision Exponentiation Function

```
      COMPLEX FUNCTION CDMPOW*16(X,Y)                                    CDPW  10
C THIS ROUTINE COMPUTES THE RESULT OF RAISING THE COMPLEX VARIABLE X TO  CDPW  20
C THE COMPLEX POWER Y. IF X AND Y HAVE ZERO IMAGINARY PARTS, THEN IT     CDPW  30
C COMPUTES THE VALUE OF X RAISED TO AN ARBITRARY REAL POWER.             CDPW  40
      COMPLEX*16 X,Y,      CDEXP,CDLOG                                   CDPW  50
      REAL*8     CDABS                                                   CDPW  60
      IF(CDABS(X)) 1,1,3                                                 CDPW  70
    3 CDMPOW=CDEXP(Y*CDLOG(X))                                           CDPW  80
      RETURN                                                             CDPW  90
    1 IF(CDABS(Y)) 2,2,4                                                 CDPW 100
    2 CDMPOW=(1.0D0,0.0D0)                                               CDPW 110
      RETURN                                                             CDPW 120
    4 CDMPOW=(0.0D0,0.0D0)                                               CDPW 130
      RETURN                                                             CDPW 140
      END                                                                CDPW 150
```

Algorithm 2a

Single Precision Gamma Function

```
      COMPLEX FUNCTION CGAMMA(Z)                                          CGAM  10
C  CGAMMA                                                                 CGAM  20
C   THIS IS A SINGLE PRECISION ROUTINE TO CALCULATE THE GAMMA FUNCTION    CGAM  30
C     ON THE COMPLEX PLANE.  THE FUNCTION RECEIVES A COMPLEX ARGUMENT,Z,  CGAM  40
C      WHICH SPECIFIES THE POINT AT WHICH THE VALUE OF THE GAMMA          CGAM  50
C     FUNCTION IS NEEDED.  THE ENTRIES  GAMMA AND IGAMMA RECEIVE REAL     CGAM  60
C     OR INTEGER ARGUMENTS RESPECTIVELY.  ARGUMENTS THAT ARE NEGATIVE     CGAM  70
C     INTEGERS OR ZERO CAUSE THE FUNCTION TO PRINT AN ERROR MESSAGE ON    CGAM  80
C     UNIT 6.                                                             CGAM  90
      COMPLEX Z,HOLD,TERM,STORE,CMPLX,GAMLOG,CEXP,CLOG,RES                CGAM 100
      REAL*4 GAMMA                                                        CGAM 110
      DIMENSION C(26),BERNOL(26)                                          CGAM 120
      DATA BERNOL/ 1.666667E-01  ,  -3.333333E-02, 2.380952E-02 , -3.333CGAM 130
     1333E-02 , 7.575757E-02 , -2.531136E-01 ,  1.166667  , -7.092157 , CGAM 140
     25.497118E01 ,  -5.291242E02 , 6.192123E03  , -8.658025E04 , 1.4255CGAM 150
     317E06 , -2.729823E07 , 6.015809E08 , -1.511632E10 , 4.296146E11 , CGAM 160
     4 -1.371166E13 , 4.883323E14  , -1.929658E16 ,  8.416930E17 , -4.03CGAM 170
     53807E19 ,  2.115075E21 , -1.208663E23  , 7.500867E24 , -5.038778E2CGAM 180
     66   /                                                              CGAM 190
      DATA C/ 1.0     ,    .5772157  , - .6558781   , - .4200264E-1 ,    CGAM 200
     1 .1665386      , - .4219774E-1 ,- .9621972E-2 , .7218943E-2 ,      CGAM 210
     2- .1165168E-02, - .2152417E-3,   .1280503E-3, - .2013486E-4,       CGAM 220
     3- .1250493E-05,   .1133027E-5, - .2056338E-6,   .6116095E-8,       CGAM 230
     4   .5002008E-8, - .1181275E-8,    .1043427E-9,  0.77823E-11,       CGAM 240
     5    -0.36968E-11,  0.5100E-12,  -0.206E-13, -0.54E-14,0.14E-14,    CGAM 250
     6 0.1E-15  /                                                        CGAM 260
      ISWTCH=1                                                            CGAM 270
   19 NUMBER=     REAL(Z)                                                 CGAM 280
      K1=0                                                                CGAM 290
      TERM=Z                                                              CGAM 300
```

Algorithm 2a (continued)

```
      IF(CABS(Z-FLOAT(NUMBER)).GT. 1.0E-6) GO TO 2                      CGAM 310
   12 HOLD=NUMBER                                                       CGAM 320
      TERM=(1.0,0.0)                                                    CGAM 330
      K1=1                                                              CGAM 340
      IF(REAL(Z).GT.0.0) GO TO 7                                        CGAM 350
      WRITE(6,1) Z                                                      CGAM 360
    1 FORMAT(1H ,'THE GAMMA FUNCTION IS NOT DEFINED FOR NEGATIVE INTERERCGAM 370
     1S OR ZERO. HENCE, ',E12.5,' , ',E12.5,' IS AN INVALID ARGUMENT.') CGAM 380
      GO TO (22,23,24),ISWTCH                                           CGAM 390
    2 IF(NUMBER) 4,5,3                                                  CGAM 400
    3 TERM=Z-NUMBER                                                     CGAM 410
      K1=1                                                              CGAM 420
      GO TO 5                                                           CGAM 430
    4 TERM=Z-NUMBER                                                     CGAM 440
      NUMBER=-NUMBER-1                                                  CGAM 450
      K1=-1                                                             CGAM 460
    5 HOLD=(0.0,0.0)                                                    CGAM 470
      IF(ABS(AIMAG(TERM)).GE.3.4)  GO TO 26                             CGAM 480
      DO 6 IBM=1,26                                                     CGAM 490
    6 HOLD=HOLD+C(IBM)*TERM**IBM                                        CGAM 500
      GO TO 7                                                           CGAM 510
   26 GAMLOG=(TERM-0.5)*CLOG(TERM) -TERM +0.9189385E+00                 CGAM 520
      DO 25 IBM=1,26                                                    CGAM 530
      RES=            BERNOL(IBM)/(2*IBM*(2*IBM-1)*TERM**(2*IBM-1))     CGAM 540
      IF(CABS(RES).LT.1.0E-08) GO TO 27                                 CGAM 550
   25 GAMLOG=GAMLOG +RES                                                CGAM 560
   27 GAMLOG=GAMLOG +RES                                                CGAM 570
      HOLD=1.0/CEXP(GAMLOG)                                             CGAM 580
    7 STORE=(1.0,0.0)                                                   CGAM 590
      IF(NUMBER.EQ.0) GO TO 9                                           CGAM 600
      DO 8 IBM=1,NUMBER                                                 CGAM 610
    8 STORE=STORE*(TERM+K1*IBM-1)                                       CGAM 620
```

Algorithm 2a (continued)

```
 9 IF(K1) 11,10,10                                                      CGAM 630
10 GO TO (14,13,15),ISWTCH                                              CGAM 640
11 GO TO (16,16,18),ISWTCH                                              CGAM 650
14 CGAMMA=STORE/HOLD                                                    CGAM 660
   RETURN                                                               CGAM 670
16 CGAMMA=1.0/(STORE*HOLD*(TERM=1.0))                                   CGAM 680
   RETURN                                                               CGAM 690
22 CGAMMA=(1.0E65,0.0E0)                                                CGAM 700
   RETURN                                                               CGAM 710
   ENTRY IGAMMA(NUMBER)                                                 CGAM 720
   IF(NUMBER.GT.14) GO TO 20                                            CGAM 730
   REALZ=NUMBER                                                         CGAM 740
   Z=CMPLX(REALZ,0.0)                                                   CGAM 750
   ISWTCH=2                                                             CGAM 760
   GO TO 12                                                             CGAM 770
20 WRITE(6,21) NUMBER                                                   CGAM 780
   RETURN                                                               CGAM 790
21 FORMAT(1H0,' INTEGER RESULTS FROM IGAMMA FOR ARGUMENTS GREATER THACGAM 800
  1N 14 OVERFLOW THE COMPUTER.',/,' THUS, AN ARGUMENT OF',I10,'  CAN CGAM 810
  2NOT BE ACCEPTED, USE GAMMA. ')                                       CGAM 820
13 REALZ=REAL(STORE/HOLD)                                               CGAM 830
   ISWTCH=REALZ                                                         CGAM 840
   IGAMMA=ISWTCH                                                        CGAM 850
   IF((REALZ-ISWTCH).GE.0.5) IGAMMA=ISWTCH+1                            CGAM 860
   RETURN                                                               CGAM 870
23 IGAMMA=9999999                                                       CGAM 880
   RETURN                                                               CGAM 890
   ENTRY GAMMA(REALZ)                                                   CGAM 900
   Z=CMPLX(REALZ,0.0)                                                   CGAM 910
   ISWTCH=3                                                             CGAM 920
   GO TO 19                                                             CGAM 930
15 GAMMA=REAL(STORE/HOLD)                                               CGAM 940
```

Algorithm 2a (continued)

```
      RETURN                                                        CGAM 950
   18 GAMMA=REAL(1.0/(STORE*HOLD*(TERM=1.0)))                       CGAM 960
      RETURN                                                        CGAM 970
   24 GAMMA=1.0E65                                                  CGAM 980
      RETURN                                                        CGAM 990
      END                                                           CGAM1000
```

Algorithm 2b

Double Precision Gamma Function

```
      COMPLEX FUNCTION CDGAMA*16(Z)                                      CDGM  10
C  CDGAMA                                                                CDGM  20
C   THIS IS A DOUBLE PRECISION ROUTINE TO CALCULATE THE GAMMA FUNCTION   CDGM  30
C     ON THE COMPLEX PLANE.  THE FUNCTION RECEIVES A COMPLEX ARGUMENT,Z, CDGM  40
C      WHICH SPECIFIES THE POINT AT WHICH THE VALUE OF THE GAMMA         CDGM  50
C     FUNCTION IS NEEDED.  THE ENTRY DGAMMA RECEIVES A REAL*8 ARGUMENT.  CDGM  60
C                                    ARGUMENTS THAT ARE NEGATIVE         CDGM  70
C     INTEGERS OR ZERO CAUSE THE FUNCTION TO PRINT AN ERROR MESSAGE ON   CDGM  80
C     UNIT 6.                                                            CDGM  90
      COMPLEX*16 Z,HOLD,TERM,STORE,DCMPLX,GAMLOG,CDEXP,CDLOG,RES         CDGM 100
      REAL*8 DREAL,DIMAG,REALZ,C(26),CDABS,DFLOAT,DLOG,BERNOL(26),DABS   CDGM 110
      DATA BERNOL/ 1.66666666666667D-01 , -3.3333333333333D-02 , 2.380952CDGM 120
     13809524D-02 , -3.3333333333333D-02 ,  7.5757575757576D-02 ,        CDGM 130
     2-2.5311355311355D-01 , 1.1666666666666D00 ,-7.0921568627451D00 ,   CDGM 140
     3 5.4971177944862D+01 ,-5.2912424242424D+02, 6.1921231884058D+03,   CDGM 150
     4-8.6580253113553D+04 , 1.4255171666667D+06,-2.7298231067816D+07,   CDGM 160
     5 6.0158087390064D+08 ,-1.1631576709 2D+10, 4.2961464306117D+11,    CDGM 170
     6-1.3711655205088D+13 , 4.8833231897359D+14,-1.9296579341940D+16,   CDGM 180
     7 8.4169304757368D+17 ,-4.0338071854059D+19, 2.1150748638082D+21,   CDGM 190
     8-1.2086626522297D+23 , 7.5008667460770D+24,-5.0387810148110D+26  /CDGM 200
      DATA C/ 1.0D0,5.7721566490153D-1,-6.5587807152025D-1,-4.2002635034CDGM 210
     1095D-2, 1.6653861138229D-1,-4.2197734555544D-2, -9.6219715278 7D-3CDGM 220
     2,7.2189432466 3D-3,-1.1651675918591D-3, -2.1524167411 9D-4,       CDGM 230
     31.2805028238 2D-4 ,-2.0134854780 7D-5, -1.2504934821D-6,          CDGM 240
     41.1330272 2D-6,-2.0563384 7D-7,6.1160 5D-9, 5.0020075D-9,         CDGM 250
     5-1.1812746D-9, 1.0434 7D-10, 7.7823D-12, -3.6968D-12, 5.10D-13,   CDGM 260
     6-2.06D-14,-5.4D-15,1.4D-15,0.1D-15/                               CDGM 270
      ISWTCH=1                                                          CDGM 280
   19 NUMBER=DREAL(Z)                                                   CDGM 290
      TERM=Z-NUMBER                                                     CDGM 300
```

Algorithm 2b (continued)

```
      TERM=Z=DFLOAT(NUMBER)                                                    CDGM 310
      TERM=CDABS(TERM)                                                         CDGM 320
      K1=0                                                                     CDGM 330
      TERM=Z                                                                   CDGM 340
      IF(CDABS(Z=DFLOAT(NUMBER)).GE.1.0D=12) GO TO 2                           CDGM 350
      HOLD=NUMBER                                                              CDGM 360
      TERM=(1.0D0,0.0D0)                                                       CDGM 370
      K1=1                                                                     CDGM 380
      IF(DREAL(Z).GT.0.0D0) GO TO 7                                            CDGM 390
      WRITE(6,1) Z                                                             CDGM 400
    1 FORMAT(1H ,'THE GAMMA FUNCTION IS NOT DEFINED FOR NEGATIVE INTERERCDGM 410
     1S OR ZERO, ',/,' HENCE, ',D20.9,' , ',D20.9,' IS AN INVALID ARGUMECDGM 420
     2NT.')                                                                    CDGM 430
      GO TO (21,22),ISWTCH                                                     CDGM 440
    2 IF(NUMBER) 4,5,3                                                         CDGM 450
    3 TERM=Z=NUMBER                                                            CDGM 460
      K1=1                                                                     CDGM 470
      GO TO 5                                                                  CDGM 480
    4 TERM=Z=NUMBER                                                            CDGM 490
      NUMBER=-NUMBER=1                                                         CDGM 500
      K1=-1                                                                    CDGM 510
    5 HOLD=(0.0D0,0.0D0)                                                       CDGM 520
      IF(DABS(DIMAG(TERM)).GE.3.4D0 ) GO TO 26                                 CDGM 530
      DO 6 IBM=1,26                                                            CDGM 540
    6 HOLD=HOLD+C(IBM)*TERM**IBM                                               CDGM 550
      GO TO 7                                                                  CDGM 560
   26 GAMLOG=(TERM=0.5)*CDLOG(TERM)=TERM +0.91893853320459D+00                 CDGM 570
      DO 25 IBM=1,26                                                           CDGM 580
      RES=          BERNOL(IBM)/(2*IBM*(2*IBM=1)*TERM**(2*IBM=1))            CDGM 590
      IF(CDABS(RES).LT.1.0D=13 ) GO TO 27                                      CDGM 600
   25 GAMLOG=GAMLOG +RES                                                       CDGM 610
   27 GAMLOG=GAMLOG +RES                                                       CDGM 620
```

Algorithm 2b (continued)

```
      HOLD=1.0D0/CDEXP(GAMLOG)                                          CDGM 630
    7 STORE=(1.0D0,0.0D0)                                               CDGM 640
      IF(NUMBER.EQ.0) GO TO 9                                           CDGM 650
      DO 8 IBM=1,NUMBER                                                 CDGM 660
    8 STORE=STORE*(TERM+K1*IBM-1)                                       CDGM 670
    9 IF(K1) 11,10,10                                                   CDGM 680
   10 GO TO (14,15),ISWTCH                                              CDGM 690
   11 GO TO (16,18),ISWTCH                                              CDGM 700
   14 CDGAMA=STORE/HOLD                                                 CDGM 710
      RETURN                                                            CDGM 720
   16 CDGAMA=1.0/(STORE*HOLD*(TERM=1.0))                                CDGM 730
      RETURN                                                            CDGM 740
   21 CDGAMA=(1.0D65,0.0D0)                                             CDGM 750
      RETURN                                                            CDGM 760
      ENTRY DGAMMA(REALZ)                                               CDGM 770
      Z=DCMPLX(REALZ,0.0D0)                                             CDGM 780
      ISWTCH=2                                                          CDGM 790
      GO TO 19                                                          CDGM 800
   15 DGAMMA=DREAL(STORE/HOLD)                                          CDGM 810
      RETURN                                                            CDGM 820
   18 DGAMMA=DREAL(1.0/(STORE*HOLD*(TERM=1.0)))                         CDGM 830
      RETURN                                                            CDGM 840
   22 DGAMMA=1.0D65                                                     CDGM 850
      RETURN                                                            CDGM 860
      END                                                               CDGM 870
```

Algorithm 3a

Single Precision Digamma Function

```
      COMPLEX FUNCTION CPSI(Z)                                          CPSI  10
C  CPSI                                                                 CPSI  20
C   THIS ROUTINE CALCULATES THE VALUE OF THE LOGARITHMIC DERIVATIVE OF  CPSI  30
C     THE GAMMA FUNCTION.  AN ASYMPTOTIC EXPANSION OF PHI FOR THE       CPSI  40
C     POSITIVE REAL PLANE >5.0 IS USED TO PREPARE THE FUNCTION.  ALL    CPSI  50
C     ARGUMENTS ARE TRANSFORMED TO THE NOTED PORTION OF THE REAL PLANE  CPSI  60
C     BY RECURSION RELATIONS.  NEGATIVE INTEGER ARGUMENTS CAUSE THIS    CPSI  70
C     ROUTINE TO PRINT AN ERROR MESSAGE ON UNIT 6.                      CPSI  80
C   THIS IS A SINGLE PRECISION ROUTINE.                                 CPSI  90
      IMPLICIT COMPLEX(A-H,O-Z)                                         CPSI 100
      REAL REAL,CABS,C(6),PSI,PI,ZREAL                                  CPSI 110
      DATA C/ .8333333E-1, -.8333333E-2,   .3968254E-2, -.4166666E-2 ,  CPSI 120
     1  .7575756E-2   ,-.2109280E-1  /                                  CPSI 130
      DATA PI/ 3.141593  /                                              CPSI 140
C THE LOGARITHMIC DERIVATIVE OF THE GAMMA FUNCTION IS UNDEFINED FOR ALL CPSI 150
C NEGATIVE INTEGERS AND ZERO.                                           CPSI 160
      NGO=1                                                             CPSI 170
   10 ZACT=Z                                                            CPSI 180
      HOLD=(0.0,0.0)                                                    CPSI 190
      STORE=(0.0,0.0)                                                   CPSI 200
      NUMBER=REAL(Z)                                                    CPSI 210
      IF(NUMBER)1,1,2                                                   CPSI 220
    1 IF(CABS(Z-NUMBER).GT. 1.0E-6) GO TO 2                             CPSI 230
C NEGATIVE INTEGER.                                                     CPSI 240
      WRITE(6,3) Z                                                      CPSI 250
    3 FORMAT(1H0,' THE LOGARITEMIC DERIVATIVE OF THE GAMMA FUNCTION IS  CPSI 260
     1 NOT DEFINED FOR NEGATIVE INTEGERS OR ZERO. ',/,' HENCE, AN ARGUMECPSI 270
     2NT OF ',2X,E15.8,' , ',E15.8,'  IS INVALID. ')                    CPSI 280
      GO TO (13,14),NGO                                                 CPSI 290
    2 IF(NUMBER) 4,5,5                                                  CPSI 300
```

Algorithm 3a (continued)

```
 4 NUMBER=-NUMBER+1                                                    CPSI 310
   ZACT=1.0-Z                                                          CPSI 320
   STORE=PI*CCOS(PI*Z)/CSIN(PI*Z)                                      CPSI 330
 5 IF(NUMBER-5)6,7,7                                                   CPSI 340
 6 JJM=5-NUMBER                                                        CPSI 350
   DO 8 IBM=1,JJM                                                      CPSI 360
 8 HOLD=HOLD+1.0/(ZACT+IBM-1)                                          CPSI 370
   ZACT=ZACT+JJM                                                       CPSI 380
 7 RESULT=0.0                                                          CPSI 390
   DO 9 IBM=1,6                                                        CPSI 400
 9 RESULT=RESULT+C(IBM)/(ZACT**(2*IBM))                                CPSI 410
   GO TO (11,12),NGO                                                   CPSI 420
11 CPSI=CLOG(ZACT)-1.0/(2.0*ZACT)-RESULT-HOLD-STORE                    CPSI 430
   RETURN                                                              CPSI 440
13  CPSI=(1.0E65,0.0)                                                  CPSI 450
   RETURN                                                              CPSI 460
   ENTRY PSI(ZREAL)                                                    CPSI 470
   Z=CMPLX(ZREAL,0.0)                                                  CPSI 480
   NGO=2                                                               CPSI 490
   GO TO 10                                                            CPSI 500
12 PSI=REAL(CLOG(ZACT)-1.0/(2.0*ZACT)-RESULT-HOLD-STORE)               CPSI 510
   RETURN                                                              CPSI 520
14  PSI=1.0E65                                                         CPSI 530
   RETURN                                                              CPSI 540
   END                                                                 CPSI 550
```

Algorithm 3b

Double Precision Digamma Function

```
      COMPLEX FUNCTION CDPSI*16(Z)                                          CDPS  10
C  CDPSI                                                                    CDPS  20
C   THIS ROUTINE CALCULATES THE VALUE OF THE LOGARITHMIC DERIVATIVE OF      CDPS  30
C     THE GAMMA FUNCTION.  AN ASYMPTOTIC EXPANSION OF PHI FOR THE           CDPS  40
C     POSITIVE REAL PLANE >5.0 IS USED TO PREPARE THE FUNCTION.  ALL        CDPS  50
C     ARGUMENTS ARE TRANSFORMED TO THE NOTED PORTION OF THE REAL PLANE      CDPS  60
C     BY RECURSION RELATIONS.  NEGATIVE INTEGER ARGUMENTS CAUSE THIS        CDPS  70
C     ROUTINE TO PRINT AN ERROR MESSAGE ON UNIT 6.                          CDPS  80
C   THIS IS A DOUBLE PRECISION ROUTINE.                                     CDPS  90
      IMPLICIT COMPLEX*16(A-H,O-Z)                                          CDPS 100
      REAL*8 DREAL,CDABS,C(11),DPSI,PI,ZREAL                                CDPS 110
      DATA C / .83333333333333D-01 , -.83333333333333D-02 ,                 CDPS 120
     1 .39682539682540D-02 , -.41666666666666D-02 ,  .75757575757576D-02CDPS 130
     2,-.21092796092796D-01, .83333333333333D-01 , -.44325980392157D+00,CDPS 140
     3 .30539543302701D+01 ,-.26456212121212D+02 ,  .28146014492754D+03/CDPS 150
      DATA PI/3.1415926535898 /                                             CDPS 160
C THE LOGARITHMIC DERIVATIVE OF THE GAMMA FUNCTION IS UNDEFINED FOR ALL     CDPS 170
C NEGATIVE INTEGERS AND ZERO.                                               CDPS 180
      NGO=1                                                                 CDPS 190
   10 ZACT=Z                                                                CDPS 200
      STORE=(0.0D0,0.0D0)                                                   CDPS 210
      HOLD=(0.0D0,0.0D0)                                                    CDPS 220
      NUMBER=DREAL(Z)                                                       CDPS 230
      IF(NUMBER)1,1,2                                                       CDPS 240
    1 IF(CDABS(Z-NUMBER).GT. 1.0D-11) GO TO 2                               CDPS 250
C NEGATIVE INTEGER.                                                         CDPS 260
      WRITE(6,3) Z                                                          CDPS 270
    3 FORMAT(1H0,' THE LOGARITEMIC DERIVATIVE OF THE GAMMA FUNCTION IS      CDPS 280
     1 NOT DEFINED FOR NEGATIVE INTEGERS OR ZERO. ',/,' HENCE, AN ARGUMECDPS 290
     2NT OF ',2X,D20.12,' , ',2X,D20.12,' IS INVALID. ')                    CDPS 300
```

Algorithm 3b (continued)

```
      GO TO (13,14),NGO                                                    CDPS 310
    2 IF(NUMBER) 4,5,5                                                     CDPS 320
    4 NUMBER=-NUMBER+1                                                     CDPS 330
      ZACT=1.0D0-Z                                                         CDPS 340
      STORE=PI*CDCOS(PI*Z)/CDSIN(PI*Z)                                     CDPS 350
    5 IF(NUMBER-5)6,7,7                                                    CDPS 360
    6 JJM=5-NUMBER                                                         CDPS 370
      DO 8 IBM=1,JJM                                                       CDPS 380
    8 HOLD=HOLD+1.0D0/(ZACT+IBM-1)                                         CDPS 390
      ZACT=ZACT+JJM                                                        CDPS 400
    7 RESULT=0.0D0                                                         CDPS 410
      DO 9 IBM=1,6                                                         CDPS 420
    9 RESULT=RESULT+C(IBM)/(ZACT**(2*IBM))                                 CDPS 430
      GO TO (11,12),NGO                                                    CDPS 440
   11 CDPSI=CDLOG(ZACT)-1.0D0/(2.0D0*ZACT)-RESULT-HOLD-STORE               CDPS 450
      RETURN                                                               CDPS 460
   13  CDPSI=(1.0D65,0.0D0)                                                CDPS 470
      RETURN                                                               CDPS 480
      ENTRY DPSI(ZREAL)                                                    CDPS 490
      Z=DCMPLX(ZREAL,0.0D0)                                                CDPS 500
      NGO=2                                                                CDPS 510
      GO TO 10                                                             CDPS 520
   14 DPSI=1.0E65                                                          CDPS 530
      RETURN                                                               CDPS 540
   12 DPSI=DREAL(CDLOG(ZACT)-1.0D0/(2.0D0*ZACT)-RESULT-HOLD-STORE)         CDPS 550
      RETURN                                                               CDPS 560
      END                                                                  CDPS 570
```

Algorithm 4a

Single Precision Hypergeometric Function For $|z|<1$

```
      COMPLEX FUNCTION CHPGEO(A,B,C,Z)                                    CHPG  10
      COMPLEX A,B,C,Z,RES,Y,CONJG,CMPLX,COMPOW,D                          CHPG  20
       DATA M,K/100,1/                                                    CHPG  30
C THE HYPERGEOMETRIC PARAMETERS ARE:                                      CHPG  40
C   A= ALPHA                                                              CHPG  50
C   B= BETA                                                               CHPG  60
C   C= GAMMA                                                              CHPG  70
C   Z= ARGUMENT                                                           CHPG  80
C RES= THE FUNCTION'S VALUE                                               CHPG  90
C      THIS ROUTINE USES THE HYPERGEOMETRIC SERIES TO CALCULATE THE       CHPG 100
C FUNCTION, THUS, THIS ROUTINE CALCULATES THE FUNCTION FOR POINTS WITHIN  CHPG 110
C THE UNIT CIRCLE OF THE COMPLEX PLANE ONLY,                              CHPG 120
      IF(CABS(Z).GE.1.0) GO TO 8                                          CHPG 130
      IF(AIMAG(C).EQ.0.0) GO TO 9                                         CHPG 140
   11 RES=(1.0,0.0)                                                       CHPG 150
      Y=(1.0,0.0)                                                         CHPG 160
      DO 1 N=1,M                                                          CHPG 170
      D=N*(C +N-1)                                                        CHPG 180
      Y=(A +N-1)*(B +N-1)              *(Y/D)*Z                           CHPG 190
      IF(CABS(Y/RES).LT.1.0E-6) GO TO 2                                   CHPG 200
      RES=RES+Y                                                           CHPG 210
    1 CONTINUE                                                            CHPG 220
      IF(K.EQ.2) GO TO 10                                                 CHPG 230
      GO TO 3                                                             CHPG 240
    2 CHPGEO=       RES                                                   CHPG 250
      IF(K.EQ.2) GO TO 10                                                 CHPG 260
      RETURN                                                              CHPG 270
    3 CHPGEO=       RES                                                   CHPG 280
      WRITE(6,4)                                                          CHPG 290
      WRITE(6,5) A ,B ,C ,Z,N                                             CHPG 300
```

Algorithm 4a (continued)

```
    4 FORMAT(1H0,' THIS IS A NOTICE OF FAILURE OF CONVERGENCE, CHPGEO HACHPG 310
     1S EXECUTED BUT THE ANSWER IS NOT CONVERGED,')                      CHPG 320
    5 FORMAT(1H ,' THE ARGUMENTS WERE: ',/,' A= ',2E15.7,' B= ',2E15.7,'CHPG 330
     1 C= ',2E15.7,/,' Z= ',2E15.7,' AFTER ',I5,' ITERATIONS,')          CHPG 340
      WRITE(6,6) RES                                                     CHPG 350
    6 FORMAT(1H ,' THE RESULT RETURNED WAS: ',2E20.12)                   CHPG 360
      RETURN                                                             CHPG 370
    9 IF(REAL(C).GT.0.0) GO TO 11                                        CHPG 380
      IC=INT(REAL(C))                                                    CHPG 390
      IF(CABS(C-IC).GT. 1.0E-6) GO TO 11                                 CHPG 400
      N=-IC                                                              CHPG 410
       IF(REAL(A).GT.0.0) GO TO 12                                       CHPG 420
      IA=INT(REAL(A))                                                    CHPG 430
      IF(CABS(A-IA).GT. 1.0E-6 ) GO TO 12                                CHPG 440
      IA=-IA                                                             CHPG 450
      IF(IA.LE.N) M=IA                                                   CHPG 460
   12 IF(REAL(B).GT.0.0) GO TO 13                                        CHPG 470
      IB=INT(REAL(B))                                                    CHPG 480
      IF(CABS(B-IB).GT. 1.0E-6 ) GO TO 13                                CHPG 490
      IB=-IB                                                             CHPG 500
      IF( IB.LE.N)                    M=IB                               CHPG 510
   13 IF(M.EQ.100) GO TO 14                                              CHPG 520
      K=2                                                                CHPG 530
                  GO TO 11                                               CHPG 540
C THE HYPERGEOMETRIC FUNCTION HAS POLES WHEN C IS A NEGATIVE INTEGER,    CHPG 550
   14 RES= 1.0E65*A*B*Z                                                  CHPG 560
   10 CHPGEO=      RES                                                   CHPG 570
      K=1                                                                CHPG 580
      M=100                                                              CHPG 590
      RETURN                                                             CHPG 600
    8 WRITE(6,7) Z                                                       CHPG 610
    7 FORMAT(1H0,' THE ARGUMENT:',E20.10,' + ',E20.10,'I IS NOT WITHIN TCHPG 620
```

Algorithm 4a (continued)

```
1HE CIRCLE OF CONVERGENCE OF THE SERIES,')                    CMPG 630
 RETURN                                                       CMPG 640
 END                                                          CMPG 650
```

Algorithm 4b

Double Precision Hypergeometric Function For $|z|<1$

```
      COMPLEX FUNCTION CDHPGM*16(A,B,C,Z)                                CDHP  10
      COMPLEX*16A,B,C,Z,RES,Y,DCONJG,ZMULT,CDMPOW,DCMPLX                 CDHP  20
      REAL*8 D,DREAL,DIMAG,CDABS,AREAL,BREAL,ZINT                        CDHP  30
       DATA M,K/100,1/                                                   CDHP  40
C THE HYPERGEOMETRIC PARAMETERS ARE:                                     CDHP  50
C   A= ALPHA                                                             CDHP  60
C   B= BETA                                                              CDHP  70
C   C= GAMMA                                                             CDHP  80
C   Z= ARGUMENT                                                          CDHP  90
C RES= THE FUNCTION'S VALUE                                              CDHP 100
C     THIS ROUTINE USES THE HYPERGEOMETRIC SERIES TO CALCULATE THE       CDHP 110
C FUNCTION, THUS, THIS ROUTINE CALCULATES THE FUNCTION FOR POINTS WITHIN CDHP 120
C THE UNIT CIRCLE OF THE COMPLEX PLANE ONLY.                             CDHP 130
      IF(CDABS(Z),GE,1,0D0) GO TO 8                                      CDHP 140
      IF(DIMAG(C),EQ,0,0D0) GO TO 9                                      CDHP 150
   11 RES=(1,0D0,0,0D0)                                                  CDHP 160
      Y=(1,0D0,0,0D0)                                                    CDHP 170
      DO 1 N=1,M                                                         CDHP 180
      D=N*(C +N-1)                                                       CDHP 190
      Y=(A +N-1)*(B +N-1)              *(Y/D)*Z                          CDHP 200
      IF(CDABS(Y/RES),LT,1,0D-11) GO TO 2                                CDHP 210
      RES=RES+Y                                                          CDHP 220
    1 CONTINUE                                                           CDHP 230
      IF(K,EQ,2) GO TO 10                                                CDHP 240
      GO TO 3                                                            CDHP 250
    2 CDHPGM=       RES                                                  CDHP 260
      IF(K,EQ,2) GO TO 10                                                CDHP 270
      RETURN                                                             CDHP 280
    3 CDHPGM=       RES                                                  CDHP 290
      WRITE(6,4)                                                         CDHP 300
```

Algorithm 4b (continued)

```
      WRITE(6,5) A ,B ,C ,Z,N                                                  CDHP 310
    4 FORMAT(1H0,' THIS IS A NOTICE OF FAILURE OF CONVERGENCE, CDHPGM HACDHP 320
     1S EXECUTED BUT THE ANSWER IS NOT CONVERGED.')                            CDHP 330
    5 FORMAT(1H ,' THE ARGUMENTS WERE:',/,' A= ',2D15.7,' B= ',2D15.7,' CDHP 340
     1C= ',2D15.7,/,' Z= ',2D15.7,' AFTER ',I5,' ITERATIONS.')                 CDHP 350
      WRITE(6,6) RES                                                           CDHP 360
    6 FORMAT(1H ,' THE RESULT RETURNED WAS: ',2D20.12)                         CDHP 370
      RETURN                                                                   CDHP 380
    9 IF(DREAL(C).GT.0.0D0) GO TO 11                                           CDHP 390
      IC=    DREAL(C)                                                          CDHP 400
      IF(CDABS(C-IC).GT.1.0D-9) GO TO 11                                       CDHP 410
      N=-IC                                                                    CDHP 420
       IF(DREAL(A).GT.0.0D0 ) GO TO 12                                         CDHP 430
      IA=   DREAL(A)                                                           CDHP 440
      IF( CDABS(A -IA) .GT. 1.0D-9)   GO TO 12                                 CDHP 450
      IA=-IA                                                                   CDHP 460
      IF(IA.LE.N) M=IA                                                         CDHP 470
   12 IF(DREAL(B) .GT. 0.0D0 ) GO TO 13                                        CDHP 480
      IB=   DREAL(B)                                                           CDHP 490
      IF(CDABS(B-IB) .GT. 1.0D-9 ) GO TO 13                                    CDHP 500
      IB=-IB                                                                   CDHP 510
      IF( IB.LE.N)                    M=IB                                     CDHP 520
   13 IF(M.EQ.100) GO TO 14                                                    CDHP 530
      K=2                                                                      CDHP 540
                 GO TO 11                                                      CDHP 550
C THE HYPERGEOMETRIC FUNCTION HAS POLES WHEN C IS A NEGATIVE INTEGER,          CDHP 560
   14 RES= 1.0D65*A*B*Z                                                        CDHP 570
   10 CDHPGM=      RES                                                         CDHP 580
      K=1                                                                      CDHP 590
      M=100                                                                    CDHP 600
      RETURN                                                                   CDHP 610
    8 WRITE(6,7) Z                                                             CDHP 620
```

Algorithm 4b (continued)

```
7 FORMAT(1H0,' THE ARGUMENT: ',D20.10,' + ',D20.10,'I IS NOT WITHIN CDHP 630
 1THE CIRCLE OF CONVERGENCE OF THE SERIES.')                        CDHP 640
  RETURN                                                            CDHP 650
  END                                                               CDHP 660
```

Algorithm 5a

Single Precision Hypergeometric Function For $|z|>1$

```
      COMPLEX FUNCTION CHPGEO(A ,B ,C ,Z )                                  CHPG  10
      IMPLICIT COMPLEX(A-H,O-Z)                                             CHPG  20
      REAL AIMAG,REAL,CABS,PSI,R,PI,GAMMA                                   CHPG  30
      DATA M,K/100,1/                                                       CHPG  40
C THIS FUNCTION CALCULATES  A SOLUTION TO THE HYPERGEOMETRIC                CHPG  50
C DIFFERENTIAL EQUATION FOR THE ENTIRE COMPLEX PLANE, THE SOLUTION          CHPG  60
C HAS POLES AT ZERO, ONE AND INFINITY ON THE REAL LINE.                     CHPG  70
C A = ALPHA                                                                 CHPG  80
C B = BETA                                                                  CHPG  90
C C = GAMMA                                                                 CHPG 100
C IT IS A COMPLEX, SINGLE PRECISION ROUTINE,                                CHPG 110
C THE FUNCTION MAY DIVERGE FOR VALUES OF A,B AND C SUCH THAT                CHPG 120
C             REAL(C-A-B)<=-1                                               CHPG 130
      DIMENSION I(6)                                                        CHPG 140
      DO 49 IBM=1,6                                                         CHPG 150
   49 I(IBM)=0,0                                                            CHPG 160
      ZMULT=(1,0,0,0)                                                       CHPG 170
C   TEST FOR INTEGERS                                                       CHPG 180
      IF((AIMAG(A),EQ,0,0),OR,(AIMAG(B),EQ,0,0),OR,(AIMAG(C),EQ,0))GO TOCHPG 190
     150                                                                    CHPG 200
      GO TO 51                                                              CHPG 210
C   A AN INTEGER?                                                           CHPG 220
   50 IF(AIMAG(A),NE,0,0) GO TO 52                                          CHPG 230
      ITEST=INT(REAL(A))                                                    CHPG 240
      IF(CABS(A-ITEST),GT, 1,0E-6 ) GO TO 52                                CHPG 250
      I(1)=1                                                                CHPG 260
      NA=ITEST                                                              CHPG 270
C   B AN INTEGER?                                                           CHPG 280
   52 IF(AIMAG(B),NE,0,0) GO TO 53                                          CHPG 290
      ITEST=INT(REAL(B))                                                    CHPG 300
```

Algorithm 5a (continued)

```
      IF(CABS(B-ITEST),GT, 1,0E-6 ) GO TO 53                                CHPG 310
      I(2)=1                                                                CHPG 320
      NB=ITEST                                                              CHPG 330
C  C AN INTEGER?                                                            CHPG 340
   53 IF(AIMAG(C),NE,0,0) GO TO 51                                          CHPG 350
      ITEST=INT(REAL(C))                                                    CHPG 360
      IF(CABS(C-ITEST),GT, 1,0E-6 ) GO TO 51                                CHPG 370
      I(3)=1                                                                CHPG 380
      NC=ITEST                                                              CHPG 390
   51 IF(CABS(Z),LT,1,0) GO TO 54                                           CHPG 400
C IF Z IS NOT WITHIN THE UNIT CIRCLE, B-A, C-A, C-B MUST BE TESTED TO       CHPG 410
C DETERMINE IF THEY ARE INTEGER,                                            CHPG 420
      STORE=B-A                                                             CHPG 430
      HOLD=C-A                                                              CHPG 440
      SHELF=C-B                                                             CHPG 450
      IF((AIMAG(STORE),NE,0,0),AND,(AIMAG(HOLD),NE,0,0),AND,(AIMAG(SHELFCHPG 460
     1),NE,0,0)) GO TO 57                                                   CHPG 470
C  B-A AN INTEGER?                                                          CHPG 480
      IF(AIMAG(STORE),NE,0,0) GO TO 55                                      CHPG 490
      ITEST=INT(REAL(STORE))                                                CHPG 500
      IF(CABS(STORE-ITEST),GT, 1,0E-6 ) GO TO 55                            CHPG 510
      I(4)=1                                                                CHPG 520
      NAMNSB=ITEST                                                          CHPG 530
C  C-A AN INTEGER?                                                          CHPG 540
   55 IF(AIMAG(HOLD),NE,0,0) GO TO 56                                       CHPG 550
      ITEST=INT(REAL(HOLD))                                                 CHPG 560
      IF(CABS(HOLD-ITEST),GT, 1,0E-6) GO TO 56                              CHPG 570
      I(5)=1                                                                CHPG 580
      NCMNSA=ITEST                                                          CHPG 590
C  C-B AN INTEGER?                                                          CHPG 600
   56 IF(AIMAG(SHELF),NE,0,0)GO TO 57                                       CHPG 610
      ITEST=INT(REAL(SHELF))                                                CHPG 620
```

Algorithm 5a (continued)

```
      IF(CABS(SHELF-ITEST).GT. 1.0E-6 ) GO TO 57                        CHPG 630
      I(6)=1                                                            CHPG 640
      NCMNSB=ITEST                                                      CHPG 650
   57 ITEST=0                                                           CHPG 660
      DO 58 IBM=1,6                                                     CHPG 670
   58 ITEST=ITEST+I(IBM)                                                CHPG 680
      IF(ITEST.NE.0) GO TO 63                                           CHPG 690
C IF THERE ARE NO INTEGER CONSTANTS OR DIFFERENCES, CALCULATE THE SERIES CHPG 700
   25 ZMULT1=CGAMMA(C)*CGAMMA(B-A)/(CGAMMA(B)*CGAMMA(C-A)*COMPOW(-Z,A)) CHPG 710
      ZMULT2=CGAMMA(C)*CGAMMA(A-B)/(CGAMMA(A)*CGAMMA(C-B)*COMPOW(-Z,B)) CHPG 720
      ZP=1.0/Z                                                          CHPG 730
C THE HYPERGEOMETRIC FUNCTION BEYOND THE UNIT CIRCLE IS A SUM OF TWO    CHPG 740
C SERIES TERMS.                                                         CHPG 750
      ALP=A                                                             CHPG 760
      BET=1.0-C+A                                                       CHPG 770
      GAM=1.0-B+A                                                       CHPG 780
      NUMBER=1                                                          CHPG 790
      GO TO 11                                                          CHPG 800
   59 F1=RES                                                            CHPG 810
      ALP=B                                                             CHPG 820
      BET=1.0-C+B                                                       CHPG 830
      GAM=1.0-A+B                                                       CHPG 840
      NUMBER=2                                                          CHPG 850
      GO TO 11                                                          CHPG 860
   60 CHPGEO=(ZMULT1*F1+ZMULT2*RES)*ZMULT                               CHPG 870
      RETURN                                                            CHPG 880
   54 ITEST=0                                                           CHPG 890
      DO 61 IBM=1,3                                                     CHPG 900
   61 ITEST=ITEST+I(IBM)                                                CHPG 910
      IF(ITEST.NE.0) GO TO 13                                           CHPG 920
C HERE, /Z/<1 AND THERE ARE NO INTEGER COEFFICIENTS,                    CHPG 930
   12 ALP=A                                                             CHPG 940
```

Algorithm 5a (continued)

```
      BET=B                                                                  CHPG 950
      GAM=C                                                                  CHPG 960
      ZP=Z                                                                   CHPG 970
   40 NUMBER=3                                                               CHPG 980
   11 RES=(1.0,0.0)                                                          CHPG 990
      Y=(1.0,0.0)                                                            CHPG1000
      IF(M.EQ.0) GO TO 62                                                    CHPG1010
      DO 1 N=1,M                                                             CHPG1020
      D=N*(GAM+N-1)                                                          CHPG1030
      Y=(ALP+N-1.0)*(BET+N-1)                    *(Y/D)*ZP                   CHPG1040
      IF(CABS(Y/RES).LT.1.0E-6) GO TO 2                                      CHPG1050
    1 RES=RES+Y                                                              CHPG1060
      IF(K.EQ.2) GO TO 62                                                    CHPG1070
      GO TO 3                                                                CHPG1080
    2 GO TO(59,60,62),NUMBER                                                 CHPG1090
    3 WRITE(6,4)                                                             CHPG1100
      WRITE(6,5) ALP,BET,GAM,ZP,N                                            CHPG1110
      WRITE(6,6) RES                                                         CHPG1120
    4 FORMAT(1H0,'THIS IS A NOTICE OF FAILURE OF CONVERGENCE, CHPGEO HASCHPG1130
     1 EXECUTED BUT THE ANSWER IS NOT CONVERGED.')                           CHPG1140
    5 FORMAT(1H ,'THE ARGUMENTS WERE: ',/,' A= ',2E16.7,' B= ',2E16.7,/,CHPG1150
     1 ' C= ',2E16.7,' Z= ',2E16.7,' AFTER ',I5,' ITERATIONS. ')             CHPG1160
    6 FORMAT(1H ,' THE RESULT RETURNED WAS: ',2E20.12)                       CHPG1170
   62 CHPGEO=ZMULT*RES                                                       CHPG1180
      K=1                                                                    CHPG1190
      M=100                                                                  CHPG1200
      RETURN                                                                 CHPG1210
C INTEGER CASES FOR /Z/<1 ARE TREATED HERE.                                  CHPG1220
   13 IF(I(3).NE.1) GO TO 12                                                 CHPG1230
      IF(NC.GT.0) GO TO 12                                                   CHPG1240
      ITEST=I(1)+I(2)                                                        CHPG1250
      IF(ITEST.NE.0) GO TO 72                                                CHPG1260
```

Algorithm 5a (continued)

```
   71 RES=   1.0E65*A*B*Z                                                CHPG1270
      GO TO 62                                                           CHPG1280
   72 K=2                                                                CHPG1290
      NC=IABS(NC)                                                        CHPG1300
      IF( I(1).EQ.0) GO TO 76                                            CHPG1310
       IF(NA.GT.0) GO TO 76                                              CHPG1320
      NA=IABS(NA)                                                        CHPG1330
      IF( NA .LE. NC) M=NA                                               CHPG1340
   76 IF( I(2).EQ.0) GO TO 74                                            CHPG1350
       IF(NB.GT.0) GO TO 74                                              CHPG1360
      NB=IABS(NB)                                                        CHPG1370
      IF(NB.LE.NC) M=NB                                                  CHPG1380
   74 IF(M.EQ. 100) GO TO 71                                             CHPG1390
      GO TO 12                                                           CHPG1400
   63 IF(I(3).EQ.1) GO TO 23                                             CHPG1410
   73 ITEST=I(1)+I(2)                                                    CHPG1420
      IF(ITEST.EQ.0) GO TO 24                                            CHPG1430
      IF(I(1).EQ.0) GO TO 18                                             CHPG1440
      IF(NA.LE.0) GO TO 12                                               CHPG1450
   18 IF(I(2).EQ.0) GO TO 24                                             CHPG1460
      IF(NB.LE.0) GO TO 12                                               CHPG1470
C ALL POSSIBLE SPECIAL CASES FOR IZI>1 ARE TREATED  HERE.                 CHPG1480
   24 ITEST =I(5)+I(6)                                                   CHPG1490
       IF(ITEST.EQ.0) GO TO 19                                           CHPG1500
      IF(I(5).EQ.0 ) GO TO 29                                            CHPG1510
      IF(NCMNSA.LT.0) GO TO 30                                           CHPG1520
   29 IF(I(6).EQ.0) GO TO 19                                             CHPG1530
      IF(NCMNSB.LT.0 ) GO TO 30                                          CHPG1540
   19 IF(I(4) .NE.1) GO TO 25                                            CHPG1550
      ITEST=I(5)+I(6)                                                    CHPG1560
      IF(ITEST.NE.2) GO TO 26                                            CHPG1570
      GO TO 37                                                           CHPG1580
```

Algorithm 5a (continued)

```
   23 IF(NC.GT.0) GO TO 73                                              CHPG1590
      ITEST=I(1)+I(2)                                                   CHPG1600
      IF(ITEST.EQ.0) GO TO 71                                           CHPG1610
      IF(CABS(Z) .GE. 1.0) GO TO 30                                     CHPG1620
      GO TO 72                                                          CHPG1630
   30 NUMBER=3                                                          CHPG1640
      IF(I(3).EQ.1) GO TO 64                                            CHPG1650
C    ONLY GAMMA-ALPHA OR GAMMA - BETA IS A NEGATIVE INTEGER, SO        CHPG1660
      GO TO 45                                                          CHPG1670
   64 CONTINUE                                                          CHPG1680
      IF(NC.GT.0) GO TO 45                                              CHPG1690
      IF(I(1).EQ.0) GO TO 65                                            CHPG1700
      IF(NA.LE.0) M=-(NC-NA)                                            CHPG1710
   65 IF(I(2) .EQ.0) GO TO 66                                           CHPG1720
      IF(NB.LE.0) M=-(NC-NB)                                            CHPG1730
   66 IF(M.EQ.100) GO TO 71                                             CHPG1740
      K=2                                                               CHPG1750
   45 ALP=C-A                                                           CHPG1760
      BET=C-B                                                           CHPG1770
      GAM=C                                                             CHPG1780
      ZMULT=COMPOW(1.0-Z,C-B-A)*ZMULT                                   CHPG1790
      ZP=Z                                                              CHPG1800
      NUMBER=3                                                          CHPG1810
      GO TO 11                                                          CHPG1820
C THIS IS FORMULA 63-18 OF THE BATEMANN MANUSCRIPT PROJECT.             CHPG1830
   26 NAMNSB=IABS(NAMNSB)                                               CHPG1840
      ALP=B                                                             CHPG1850
      IF(REAL(B-A).GE.0.0) ALP=A                                        CHPG1860
      SHELF=(1.0,0.0)                                                   CHPG1870
      STORE=CLOG(-Z)                                                    CHPG1880
      IF(NAMNSB.EQ.0) GO TO 22                                          CHPG1890
      DO 95 IBM=1,NAMNSB                                                CHPG1900
```

Algorithm 5a (continued)

```
   95 SHELF=SHELF*(ALP+IBM-1)*(ALP-C+IBM)/IBM                                CHPG1910
   22 HOLD =SHELF*(STORE+PSI(1,0+NAMNSB)+PSI(1,0)-CPSI(ALP+NAMNSB)-CPSI(CHPG1920
     1C-ALP-NAMNSB))                                                        CHPG1930
      DO 87 IBM=1,100                                                     CHPG1940
      NA=NAMNSB+IBM                                                       CHPG1950
      SHELF=SHELF*(ALP+NA -1,0    )*(    -C+ALP+NA          )/(IBM*(NA    CHPG1960
     1  )*Z )                                                             CHPG1970
      RES=SHELF  *(STORE+ PSI(1,0+NA          )+ PSI(1,0+IBM)-CPSI(ALP+NA CHPG1980
     2       )-CPSI(C-ALP-NA          ))                                 CHPG1990
      IF(CABS( RES /HOLD) .LT.1.0E-6) GO TO 42                            CHPG2000
   87 HOLD=HOLD+RES                                                       CHPG2010
   42 CONTINUE                                                            CHPG2020
      IF(NAMNSB.LT.2 ) GO TO 43                                           CHPG2030
      STORE=GAMMA(NAMNSB+0.0)/CGAMMA(C-ALP)                               CHPG2040
      SHELF=(1.0   ,0.0)                                                  CHPG2050
      N=NAMNSB-1                                                          CHPG2060
      DO 96 IBM=1,N                                                       CHPG2070
      SHELF=SHELF*(ALP+IBM-1.0) /(IBM*Z      )                            CHPG2080
   96 STORE=STORE+SHELF* GAMMA(NAMNSB-IBM+0.0 )/CGAMMA(C-ALP-IBM)         CHPG2090
      GO TO 44                                                            CHPG2100
   43 STORE=NAMNSB                        /CGAMMA(C-ALP)                  CHPG2110
C HOLD AND STORE HOLD THE FIRST AND SECOND SERIES RESPECTIVELY FOR         CHPG2120
C FORMULA 63-18 OF THE BATEMAN MANUSCRIPT PROJECT, VOL. I.                CHPG2130
   44 SHELF=CGAMMA(C)/(COMPOW(-Z,ALP)*CGAMMA(ALP+NAMNSB))                 CHPG2140
      CHPGEO=SHELF*(HOLD/(CGAMMA(C-ALP)*(-Z)**NAMNSB)+STORE)              CHPG2150
      RETURN                                                              CHPG2160
C THIS IS FORMULA 63-19 OF THE BATEMANN MANUSCRIPT PROJECT.               CHPG2170
   37 ALP=B                                                               CHPG2180
      IF(REAL(B-A).GT.0.0) ALP=A                                          CHPG2190
      NAMNSB=IABS(NAMNSB)                                                 CHPG2200
      ITEST=-NAMNSB+INT(REAL(C-ALP))                                      CHPG2210
      IF(ITEST.LT.0) GO TO 26                                             CHPG2220
```

Algorithm 5a (continued)

```
      STORE=CLOG(-Z)                                                    CHPG2230
      NB=NAMNSB+ITEST                                                   CHPG2240
       NC=NAMNSB -1                                                     CHPG2250
      HOLD=ALP*(1.0-(      NB      ))                                   CHPG2260
      IF(NAMNSB.EQ.0) HOLD=(1.0,0.0)                                    CHPG2270
      IF(ITEST.LE.0) HOLD=(0.0,0.0)                                     CHPG2280
      IF(NAMNSB.LE.1) GO TO 39                                          CHPG2290
      DO 31 IBM=1,NC                                                    CHPG2300
   31 HOLD=HOLD*(ALP+IBM)*(1.0-       NB       +IBM)/(IBM+1)           CHPG2310
   39 R=ITEST                                                           CHPG2320
      SHELF=HOLD*(STORE+PSI(1.0+NAMNSB)+ PSI(1.0)-CPSI(ALP+NAMNSB)- PSI(CHPG2330
     1R    ))                                                           CHPG2340
      NA=ITEST-1                                                        CHPG2350
      IF(ITEST.LE.1) GO TO 98                                           CHPG2360
C THIS IS THE L SERIES.                                                 CHPG2370
      DO 99 IBM=1,NA                                                    CHPG2380
      R=ITEST-IBM                                                       CHPG2390
      HOLD=HOLD*(ALP+IBM-1+NAMNSB)*(IBM-ITEST)/(IBM*(IBM+NAMNSB)*Z)     CHPG2400
      RES= HOLD                                                         CHPG2410
     1 *(STORE+PSI(1.0+NAMNSB+IBM)+PSI(1.0+IBM)-CPSI(ALP+NAMNSB+IBM)    CHPG2420
     2 -PSI(R))                                                         CHPG2430
   99 SHELF=SHELF +RES                                                  CHPG2440
   98 SHELF=SHELF/((-Z)**NAMNSB*IGAMMA(NB))                             CHPG2450
      GAM=(1.0,0.0 )                                                    CHPG2460
      STORE=(1.0,0.0)                                                   CHPG2470
      IF( ITEST .LE.0.0) GO TO 33                                       CHPG2480
      NA=NAMNSB                                                         CHPG2490
      IF(NAMNSB.EQ.0) NA=NA+1                                           CHPG2500
C PRESET CONSTANTS FOR M AND INFINITE SERIES, GAM FOR INFINITE SERIES,  CHPG2510
      DO 32 IBM=1,ITEST                                                 CHPG2520
      GAM=GAM*(ALP+IBM-1.0) /IBM**2                                     CHPG2530
      STORE=STORE/(IBM+NA    -1.0)                                      CHPG2540
```

Algorithm 5a (continued)

```
   32  NA=NAMNSB                                                          CHPG2550
   33 GAM= GAM/Z**ITEST                                                   CHPG2560
      HOLD=STORE                                                          CHPG2570
      IF(NAMNSB.LE.1) GO TO 34                                            CHPG2580
      DO 35 IBM=1,NC                                                      CHPG2590
      GAM=GAM*(ALP+ITEST+IBM-1.0)/(ITEST+IBM)                             CHPG2600
      STORE=STORE*(NB-IBM)*(ALP+IBM-1.0)/((NAMNSB-IBM)*IBM*Z)             CHPG2610
   35 HOLD=HOLD+STORE                                                     CHPG2620
      GAM=GAM*(ALP+NB-1.0)/NB                                             CHPG2630
      GO TO 41                                                            CHPG2640
   34 IF(NAMNSB.EQ.0) HOLD=(0.0,0.0,0.0)                                  CHPG2650
      IF(NAMNSB.EQ.1) GAM=(ALP+ITEST)*GAM/(ITEST+1.0)                     CHPG2660
   41 STORE=GAM                                                           CHPG2670
C THIS IS THE INFINITE SERIES.                                            CHPG2680
      DO 36 IBM=1,100                                                     CHPG2690
      GAM=GAM*(ALP+NB+IBM-1.0)*IBM/((NB+IBM)*(ITEST+IBM)*Z)               CHPG2700
      IF(CABS(GAM/STORE) .LT. 1.0E-06) GO TO 38                           CHPG2710
   36 STORE=STORE+GAM                                                     CHPG2720
   38 CONTINUE                                                            CHPG2730
      STORE=(-1)**NB*STORE/(-Z)**NAMNSB                                   CHPG2740
      BET=CGAMMA(ALP+NB)/(CGAMMA(ALP+NAMNSB)*COMPOW(-Z,ALP))              CHPG2750
      CHPGEO=BET*(STORE+HOLD+SHELF)                                       CHPG2760
      RETURN                                                              CHPG2770
      END                                                                 CHPG2780
```

Algorithm 5b

Double Precision Hypergeometric Function For $|z|>1$

```
      COMPLEX FUNCTION CDHPGO(A,B,C,Z)                                  CDHG  10
      IMPLICIT COMPLEX*16 (A-H,O-Z)                                     CDHG  20
      DOUBLE PRECISION CDABS,DREAL,DIMAG,DPSI,DGAMMA                    CDHG  30
      DATA M,K/100,1/                                                   CDHG  40
C THIS FUNCTION CALCULATES  A SOLUTION TO THE HYPERGEOMETRIC            CDHG  50
C DIFFERENTIAL EQUATION FOR THE ENTIRE COMPLEX PLANE. THE SOLUTION      CDHG  60
C HAS POLES AT ZERO, ONE AND INFINITY ON THE REAL LINE.                 CDHG  70
C A = ALPHA                                                             CDHG  80
C B = BETA                                                              CDHG  90
C C = GAMMA                                                             CDHG 100
C IT IS A COMPLEX, SINGLE PRECISION ROUTINE.                            CDHG 110
C THE FUNCTION MAY DIVERGE FOR VALUES OF A,B AND C SUCH THAT            CDHG 120
C            REAL(C-A-B)<=-1                                            CDHG 130
      DIMENSION I(6)                                                    CDHG 140
      DO 49 IBM=1,6                                                     CDHG 150
   49 I(IBM)=0                                                          CDHG 160
      ZMULT=(1.0D0,0.0D0)                                               CDHG 170
C   TEST FOR INTEGERS                                                   CDHG 180
      IF( (DIMAG(A).EQ.0.0D0) .OR. (DIMAG(B).EQ. 0.0D0) .OR.            CDHG 190
     1 (DIMAG(C) .EQ. 0.0D0) ) GO TO 50                                 CDHG 200
      GO TO 51                                                          CDHG 210
C   A AN INTEGER?                                                       CDHG 220
   50 IF( DIMAG(A) .NE. 0.0D0) GO TO 52                                 CDHG 230
      ITEST= DREAL(A)                                                   CDHG 240
      IF( CDABS(A-ITEST).GT. 1.0D-11) GO TO 52                          CDHG 250
      I(1)=1                                                            CDHG 260
      NA=ITEST                                                          CDHG 270
C   B AN INTEGER?                                                       CDHG 280
   52 IF( DIMAG(B) .NE. 0.0D0) GO TO 53                                 CDHG 290
      ITEST= DREAL(B)                                                   CDHG 300
```

Algorithm 5b (continued)

```
      IF( CDABS(B-ITEST).GT. 1.0D-11) GO TO 53                          CDHG 310
      I(2)=1                                                            CDHG 320
      NB=ITEST                                                          CDHG 330
C   C AN INTEGER?                                                       CDHG 340
   53 IF( DIMAG(C).NE. 0.0D0 ) GO TO 51                                 CDHG 350
      ITEST= DREAL(C)                                                   CDHG 360
      IF( CDABS(C-ITEST) .GT. 1.0D-11) GO TO 51                         CDHG 370
      I(3)=1                                                            CDHG 380
      NC=ITEST                                                          CDHG 390
   51 IF( CDABS(Z) .LT. 1.0D0) GO TO 54                                 CDHG 400
C IF Z IS NOT WITHIN THE UNIT CIRCLE, B-A, C-A, C-B MUST BE TESTED TO   CDHG 410
C DETERMINE IF THEY ARE INTEGER.                                        CDHG 420
      STORE=B-A                                                         CDHG 430
      HOLD=C-A                                                          CDHG 440
      SHELF=C-B                                                         CDHG 450
      IF( (DIMAG(STORE).NE. 0.0D0) .AND. (DIMAG(HOLD) .NE. 0.0D0)       CDHG 460
     1  .AND. (DIMAG(SHELF) .NE. 0.0D0 )) GO TO 57                      CDHG 470
C   B-A AN INTEGER?                                                     CDHG 480
      IF( DIMAG(STORE) .NE. 0.0D0) GO TO 55                             CDHG 490
      ITEST= DREAL(STORE)                                               CDHG 500
      IF( CDABS(STORE-ITEST) .GT. 1.0D-11) GO TO 55                     CDHG 510
      I(4)=1                                                            CDHG 520
      NAMNSB=ITEST                                                      CDHG 530
C   C-A AN INTEGER?                                                     CDHG 540
   55 IF( DIMAG(HOLD) .NE. 0.0D0) GO TO 56                              CDHG 550
      ITEST= DREAL(HOLD)                                                CDHG 560
      IF( CDABS(HOLD-ITEST) .GT. 1.0D-11 ) GO TO 56                     CDHG 570
      I(5)=1                                                            CDHG 580
      NCMNSA=ITEST                                                      CDHG 590
C   C-B AN INTEGER?                                                     CDHG 600
   56 IF( DIMAG(SHELF) .NE. 0.0D0) GO TO 57                             CDHG 610
      ITEST= DREAL(SHELF)                                               CDHG 620
```

Algorithm 5b (continued)

```
      IF( CDABS(SHELF-ITEST) .GT. 1.0D-11) GO TO 57                          CDHG 630
      I(6)=1                                                                 CDHG 640
      NCMNSB=ITEST                                                           CDHG 650
   57 ITEST=0                                                                CDHG 660
      DO 58 IBM=1,6                                                          CDHG 670
   58 ITEST=ITEST+I(IBM)                                                     CDHG 680
      IF(ITEST.NE.0) GO TO 63                                                CDHG 690
C IF THERE ARE NO INTEGER CONSTANTS OR DIFFERENCES, CALCULATE THE SERIES     CDHG 700
   25 ZMULT1= CDGAMA(C)*CDGAMA(B-A)/(CDGAMA(B)*CDGAMA(C-A)*CDMPOW(-Z,A))     CDHG 710
      ZMULT2=CDGAMA(C)*CDGAMA(A-B)/(CDGAMA(A)*CDGAMA(C-B)*CDMPOW(-Z,B))      CDHG 720
      ZP= 1.0D0/ Z                                                           CDHG 730
C THE HYPERGEOMETRIC FUNCTION BEYOND THE UNIT CIRCLE IS A SUM OF TWO         CDHG 740
C SERIES TERMS,                                                              CDHG 750
      ALP=A                                                                  CDHG 760
      BET=1.0D0-C+A                                                          CDHG 770
      GAM=1.0D0-B+A                                                          CDHG 780
      NUMBER=1                                                               CDHG 790
      GO TO 11                                                               CDHG 800
   59 F1=RES                                                                 CDHG 810
      ALP=B                                                                  CDHG 820
      BET=1.0D0-C+B                                                          CDHG 830
      GAM=1.0D0-A+B                                                          CDHG 840
      NUMBER=2                                                               CDHG 850
      GO TO 11                                                               CDHG 860
   60 CDHPGO=(ZMULT1*F1+ZMULT2*RES)*ZMULT                                    CDHG 870
      RETURN                                                                 CDHG 880
   54 ITEST=0                                                                CDHG 890
      DO 61 IBM=1,3                                                          CDHG 900
   61 ITEST=ITEST+I(IBM)                                                     CDHG 910
      IF(ITEST.NE.0) GO TO 13                                                CDHG 920
C HERE, /Z/<1 AND THERE ARE NO INTEGER COEFFICIENTS,                         CDHG 930
   12 ALP=A                                                                  CDHG 940
```

Algorithm 5b (continued)

```
      BET=B                                                              CDHG 950
      GAM=C                                                              CDHG 960
      ZP=Z                                                               CDHG 970
   40 NUMBER=3                                                           CDHG 980
   11 RES= (1.0D0, 0.0D0)                                                CDHG 990
      Y= (1.0D0, 0.0D0)                                                  CDHG1000
      IF(M.EQ.0 ) GO TO 62                                               CDHG1010
      DO 1 N=1,M                                                         CDHG1020
      D=N*(GAM+N-1)                                                      CDHG1030
      Y=(ALP+N-1.0)*(BET+N-1)                    *(Y/D)*ZP               CDHG1040
      IF( CDABS(Y/RES) .LT. 1.0D-11) GO TO 2                             CDHG1050
    1 RES=RES+Y                                                          CDHG1060
      IF(K.EQ.2) GO TO 62                                                CDHG1070
      GO TO 3                                                            CDHG1080
    2 GO TO(59,60,62),NUMBER                                             CDHG1090
    3 WRITE(6,4)                                                         CDHG1100
      WRITE(6,5) ALP,BET,GAM,ZP,N                                        CDHG1110
      WRITE(6,6) RES                                                     CDHG1120
    4 FORMAT(1H0,'THIS IS A NOTICE OF FAILURE OF CONVERGENCE. CHPGEO HASCDHG1130
     1 EXECUTED BUT THE ANSWER IS NOT CONVERGED.')                       CDHG1140
    5 FORMAT(1H ,' THE ARGUMENTS WERE: ',/,' A= ',2D16.7,' B= ',2D16.7,/CDHG1150
     1,' C= ',2D16.7,' Z= ',2D16.7,' AFTER ',I4,' ITERATIONS.')          CDHG1160
    6 FORMAT(1H ,' THE RESULT RETURNED WAS: ',2D20.12)                   CDHG1170
   62 CDHPGO=ZMULT*RES                                                   CDHG1180
      K=1                                                                CDHG1190
      M=100                                                              CDHG1200
      RETURN                                                             CDHG1210
C INTEGER CASES FOR /Z/<1 ARE TREATED HERE.                              CDHG1220
   13 IF(I(3).NE.1) GO TO 12                                             CDHG1230
      IF(NC.GT.0) GO TO 12                                               CDHG1240
      ITEST=I(1)+I(2)                                                    CDHG1250
      IF(ITEST.NE.0) GO TO 72                                            CDHG1260
```

Algorithm 5b (continued)

```
   71 RES=   1.0E65*A*B*Z                                                CDHG1270
      GO TO 62                                                           CDHG1280
   72 K=2                                                                CDHG1290
      NC=IABS(NC)                                                        CDHG1300
      IF( I(1).EQ.0) GO TO 76                                            CDHG1310
       IF(NA.GT.0) GO TO 76                                              CDHG1320
      NA=IABS(NA)                                                        CDHG1330
      IF( NA .LE. NC) M=NA                                               CDHG1340
   76 IF( I(2).EQ.0) GO TO 74                                            CDHG1350
       IF(NB.GT.0) GO TO 74                                              CDHG1360
      NB=IABS(NB)                                                        CDHG1370
      IF(NB.LE.NC) M=NB                                                  CDHG1380
   74 IF(M.EQ. 100) GO TO 71                                             CDHG1390
      GO TO 12                                                           CDHG1400
   63 IF(I(3).EQ.1) GO TO 23                                             CDHG1410
   73 ITEST=I(1)+I(2)                                                    CDHG1420
      IF(ITEST.EQ.0) GO TO 24                                            CDHG1430
      IF(I(1).EQ.0) GO TO 18                                             CDHG1440
      IF(NA.LE.0) GO TO 12                                               CDHG1450
   18 IF(I(2).EQ.0) GO TO 24                                             CDHG1460
      IF(NB.LE.0) GO TO 12                                               CDHG1470
C ALL POSSIBLE SPECIAL CASES FOR IZI>1 ARE TREATED  HERE.                CDHG1480
   24 ITEST =I(5)+I(6)                                                   CDHG1490
       IF(ITEST.EQ.0) GO TO 19                                           CDHG1500
      IF(I(5).EQ.0 ) GO TO 29                                            CDHG1510
      IF(NCMNSA.LT.0) GO TO 30                                           CDHG1520
   29 IF(I(6).EQ.0) GO TO 19                                             CDHG1530
      IF(NCMNSB.LT.0 ) GO TO 30                                          CDHG1540
   19 IF(I(4) .NE.1) GO TO 25                                            CDHG1550
      ITEST=I(5)+I(6)                                                    CDHG1560
      IF(ITEST.NE.2) GO TO 26                                            CDHG1570
      GO TO 37                                                           CDHG1580
```

Algorithm 5b (continued)

```
   23 IF(NC.GT.0) GO TO 73                                                CDHG1590
      ITEST=I(1)+I(2)                                                     CDHG1600
      IF(ITEST.EQ.0) GO TO 71                                             CDHG1610
      IF(CDABS(Z).GE. 1.0D0) GO TO 30                                     CDHG1620
      GO TO 72                                                            CDHG1630
   30 NUMBER=3                                                            CDHG1640
      IF(I(3).EQ.1) GO TO 64                                              CDHG1650
C    ONLY GAMMA=ALPHA OR GAMMA = BETA IS A NEGATIVE INTEGER, SO           CDHG1660
      GO TO 45                                                            CDHG1670
   64 CONTINUE                                                            CDHG1680
      IF(NC.GT.0) GO TO 45                                                CDHG1690
      IF(I(1).EQ.0) GO TO 65                                              CDHG1700
      IF(NA.LE.0) M=-(NC-NA)                                              CDHG1710
   65 IF(I(2) .EQ.0) GO TO 66                                             CDHG1720
      IF(NB.LE.0) M=-(NC-NB)                                              CDHG1730
   66 IF(M.EQ.100) GO TO 71                                               CDHG1740
      K=2                                                                 CDHG1750
   45 ALP=C-A                                                             CDHG1760
      BET=C-B                                                             CDHG1770
      GAM=C                                                               CDHG1780
      ZMULT= CDMPOW(1.0D0-Z, C-B-A) *ZMULT                                CDHG1790
      ZP=Z                                                                CDHG1800
      NUMBER=3                                                            CDHG1810
      GO TO 11                                                            CDHG1820
C THIS IS FORMULA 63-18 OF THE BATEMANN MANUSCRIPT PROJECT,               CDHG1830
   26 NAMNSB=IABS(NAMNSB)                                                 CDHG1840
      ALP=B                                                               CDHG1850
      IF( DREAL(B-A) .GE. 0.0D0) ALP=A                                    CDHG1860
      SHELF= (1.0D0, 0.0D0)                                               CDHG1870
      STORE= CDLOG(-Z)                                                    CDHG1880
      IF(NAMNSB.EQ.0) GO TO 22                                            CDHG1890
      DO 95 IBM=1,NAMNSB                                                  CDHG1900
```

Algorithm 5b (continued)

```
   95 SHELF=SHELF*(ALP+IBM-1)*(ALP-C+IBM)/IBM                                CDHG1910
   22 HOLD= SHELF*( STORE+ DPSI(1.0D0 +NAMNSB) + DPSI(1.0D0)- CDPSI(ALP CDHG1920
     1+NAMNSB)- CDPSI( C-ALP-NAMNSB))                                       CDHG1930
      DO 87 IBM=1,100                                                       CDHG1940
      NA=NAMNSB+IBM                                                         CDHG1950
      SHELF=SHELF*(ALP+NA -1.0    )*(    -C+ALP+NA          )/(IBM*(NA      CDHG1960
     1   )*Z )                                                              CDHG1970
      RES= SHELF*(STORE+DPSI(1.0D0+NA) +DPSI(1.0D0+IBM)-CDPSI(ALP+NA) - CDHG1980
     1 CDPSI( C-ALP-NA))                                                    CDHG1990
      IF(CDABS( RES/HOLD) .LT. 1.0D-11) GO TO 42                            CDHG2000
   87 HOLD=HOLD+RES                                                         CDHG2010
   42 CONTINUE                                                              CDHG2020
      IF(NAMNSB.LT.2 ) GO TO 43                                             CDHG2030
      STORE= DGAMMA( NAMNSB + 0.0D0)/CDGAMA(C-ALP)                          CDHG2040
      SHELF =(1.0D0,0.0D0)                                                  CDHG2050
      N=NAMNSB-1                                                            CDHG2060
      DO 96 IBM=1,N                                                         CDHG2070
      SHELF=SHELF*(ALP+IBM-1.0) /(IBM*Z      )                              CDHG2080
   96 STORE= STORE +SHELF* DGAMMA(NAMNSB- IBM+0.0D0)/CDGAMA(C-ALP-IBM)      CDHG2090
      GO TO 44                                                              CDHG2100
   43 STORE= NAMNSB/CDGAMA(C-ALP)                                           CDHG2110
C HOLD AND STORE HOLD THE FIRST AND SECOND SERIES RESPECTIVELY FOR          CDHG2120
C FORMULA 63-18 OF THE BATEMAN MANUSCRIPT PROJECT, VOL. I.                 CDHG2130
   44 SHELF=CDGAMA(C)/(CDMPOW(-Z,ALP)*CDGAMA(ALP+NAMNSB))                   CDHG2140
      CDHPGO=SHELF*(HOLD/(CDGAMA(C-ALP)*(-Z) **NAMNSB)+STORE)               CDHG2150
      RETURN                                                                CDHG2160
C THIS IS FORMULA 63-19 OF THE BATEMANN MANUSCRIPT PROJECT.                 CDHG2170
   37 ALP=B                                                                 CDHG2180
      IF( DREAL(B-A) .GT. 0.0D0) ALP=A                                      CDHG2190
      NAMNSB=IABS(NAMNSB)                                                   CDHG2200
      ITEST= -NAMNSB+ DREAL(C-ALP)                                          CDHG2210
      IF(ITEST.LT.0) GO TO 26                                               CDHG2220
```

Algorithm 5b (continued)

```
      STORE= CDLOG(-Z)                                                    CDHG2230
      NB=NAMNSB+ITEST                                                     CDHG2240
       NC=NAMNSB -1                                                       CDHG2250
      HOLD=ALP*(1.0-(      NB      ))                                     CDHG2260
      IF( NAMNSB.EQ. 0) HOLD= (1.0D0,0.0D0)                               CDHG2270
      IF( ITEST .LE. 0) HOLD= (0.0D0,0.0D0)                               CDHG2280
      IF(NAMNSB.LE.1) GO TO 39                                            CDHG2290
      DO 31 IBM=1,NC                                                      CDHG2300
   31 HOLD=HOLD*(ALP+IBM)*(1.0-       NB       +IBM)/(IBM+1)             CDHG2310
   39 R=ITEST                                                             CDHG2320
      SHELF=HOLD*(STORE +DPSI(1.0D0+NAMNSB)+ DPSI(1.0D0)- CDPSI(ALP+      CDHG2330
     1 NAMNSB)- DPSI(R))                                                 CDHG2340
      NA=ITEST-1                                                          CDHG2350
      IF(ITEST.LE.1) GO TO 98                                             CDHG2360
C THIS IS THE L SERIES.                                                   CDHG2370
      DO 99 IBM=1,NA                                                      CDHG2380
      R=ITEST-IBM                                                         CDHG2390
      HOLD=HOLD*(ALP+IBM-1+NAMNSB)*(IBM-ITEST)/(IBM*(IBM+NAMNSB)*Z)       CDHG2400
      RES= HOLD*(STORE +DPSI(1.0D0+NAMNSB+IBM)+ DPSI(1.0D0+IBM) -         CDHG2410
     1 CDPSI(ALP+ NAMNSB+IBM) -DPSI(R))                                   CDHG2420
   99 SHELF=SHELF +RES                                                    CDHG2430
   98 SHELF= SHELF/((-Z)**NAMNSB*DGAMMA(NB+0.0D0))                        CDHG2440
      GAM=(1.0,0.0 )                                                      CDHG2450
      STORE=(1.0,0.0)                                                     CDHG2460
      IF( ITEST .LE.0.0) GO TO 33                                         CDHG2470
      NA=NAMNSB                                                           CDHG2480
      IF(NAMNSB.EQ.0) NA=NA+1                                             CDHG2490
C PRESET CONSTANTS FOR M AND INFINITE SERIES, GAM FOR INFINITE SERIES,    CDHG2500
      DO 32 IBM=1,ITEST                                                   CDHG2510
      GAM=GAM*(ALP+IBM-1.0) /IBM**2                                       CDHG2520
      STORE=STORE/(IBM+NA    -1.0)                                        CDHG2530
   32  NA=NAMNSB                                                          CDHG2540
```

Algorithm 5b (continued)

```
   33 GAM= GAM/Z**ITEST                                                    CDHG2550
      HOLD=STORE                                                           CDHG2560
      IF(NAMNSB.LE.1) GO TO 34                                             CDHG2570
      DO 35 IBM=1,NC                                                       CDHG2580
      GAM=GAM*(ALP+ITEST+IBM-1.0)/(ITEST+IBM)                              CDHG2590
      STORE=STORE*(NB-IBM)*(ALP+IBM-1.0)/((NAMNSB-IBM)*IBM*Z)              CDHG2600
   35 HOLD=HOLD+STORE                                                      CDHG2610
      GAM=GAM*(ALP+NB-1.0)/NB                                              CDHG2620
      GO TO 41                                                             CDHG2630
   34 IF(NAMNSB.EQ.0) HOLD=(0.0,0.0)                                       CDHG2640
      IF(NAMNSB.EQ.1) GAM=(ALP+ITEST)*GAM/(ITEST+1.0)                      CDHG2650
   41 STORE=GAM                                                            CDHG2660
C THIS IS THE INFINITE SERIES.                                             CDHG2670
      DO 36 IBM=1,100                                                      CDHG2680
      GAM=GAM*(ALP+NB+IBM-1.0)*IBM/((NB+IBM)*(ITEST+IBM)*Z)                CDHG2690
      IF( CDABS(GAM/STORE) .LT. 1.0D-11 ) GO TO 38                         CDHG2700
   36 STORE=STORE+GAM                                                      CDHG2710
   38 CONTINUE                                                             CDHG2720
      STORE=(-1)**NB*STORE/(-Z)**NAMNSB                                    CDHG2730
      BET= CDGAMA(ALP+NB)/(CDGAMA(ALP+NAMNSB)*CDMPOW(-Z,ALP))              CDHG2740
      CDHPGO=BET*(STORE+HOLD+SHELF)                                        CDHG2750
      RETURN                                                               CDHG2760
      END                                                                  CDHG2770
```

Part II

The Method Of Subtracted Asymptotics

1: Introduction

Efforts to solve the quantum equations governing the collision of three atoms below the three-separated-atom threshold are generally centered about some specialized technique for solving second order, linear, partial differential equations in a small, bounded geometry. The study of quantum effects in chemical reactions described here, follows this pattern in that it is predominately a study of a method for solving the three-atom Schrödinger equation rather than a study of the three-atom collision itself.

The concentration on methods, whenever an attempt is made to solve the three-atom collision equations with a minimum of approximations, is brought about by the complexity of the equations and the poor state of numerical solution techniques. Extended studies of quantum effects in chemical reactions can only be undertaken once the difficulties of time and cost which currently plague such studies are resolved.

The study of the Method of Subtracted Asymptotics (M. S. A.) was undertaken in a search for mechanisms which would resolve the numerical restraints currently blocking the investigation of reactive collisions.

Historical Background

The Method of Subtracted Asymptotics developed from a symbiotic interaction between two research groups. One of the basic concepts of this technique was developed by F. S. Levin who was attempting to solve electron-hydrogen scattering problems at

Brookhaven National Laboratory. Levin proposed (Le65) (Le66a), that the incoming flux or source term be subtracted out of the total solution of the scattering equations. Both of the original papers by Levin were a formal treatment of atom-electron scattering in which the sectioning of the solution into a source part and a scattered part served only to identify the roles played by these elements of the solution in the scattering equations.

The suggestion that the scattering wavefunction be broken into parts was selected as a fundamental tool for solving the scattering equations by the research group of B. N. Zakhariev* at the Joint Institute for Nuclear Research, Dubna, U. S. S. R. In their earliest work (Am66) on a formalism that evolved into the Method of Subtracted Asymptotics, Amirkhanov, Zhigunov and Zakhariev proposed that the asymptotic behavior of reacted fragments of the total reactive collision solution be subtracted out of the complete wavefunction and the remaining portion of the solution be treated as the wavefunction for an inelastic collision problem.

Both Levin and Zakhariev et al (Le66b, Ef67a) applied the solution sectioning proposal to the problem of developing solutions which obeyed the Pauli Principle for identical particle collisions. Thereafter, Zakhariev and coworkers adopted their formulation of Levin's original concept as a general mechanism for treating reactive systems.

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*Other possible translations are: B. N. Zakharev, B. N. Zakhar'ev, B. N. Zakharye and B. N. Zakharyev.

Despite their dependence on the concept of sectioning the scattering solution, the equations of Levin and Zakhariev differ in several respects. Levin's work concentrates on subtracting out the incoming, entrance channel flux, thus creating coupled integral equations which he proposes to solve iteratively. Zakhariev removes all rearranged particle configurations from the total solution to yield a set of equations which demand a single channel, one configuration function to satisfy them. Zakhariev then proposes to expand this function in eigenfunctions obtained from the asymptotic potential of the single rearrangement channel for which his function is created.

Additional treatment of the equations for removing altered configurations from the total scattering solution lead to a complete set of equations which Efimenko, Zhigunov and Zakhariev (Ef67b) presented as a general method for solving scattering problems involving rearrangements of the target.

The Method of Subtracted Asymptotics was published in several journals (Za67, Ef68a, Ef68b) after being sectionally described in the research reports cited above. The historical development of the Method of Subtracted Asymptotics fragments after the publication of the technique. To clarify the proposals which constitute M. S. A., the equations from referance Ef68b will be presented here. This will predicate the detailed analysis of the formalism contained in later sections.

Let α or β denote possible bonding configurations of the

three atoms of Figure 1. The eigenfunctions of each diatom in any of the possible configurations, α, will be defined by

$$h_\alpha \phi_i^\alpha = \epsilon_i^\alpha \phi_i^\alpha \ .$$

The total solution to the reactive scattering problem will be Ψ. Prepare another function Φ such that

$$\text{Lim}\,\Phi = \begin{cases} 0 & \text{for } R_\alpha \to \infty, \\ \lim \Psi & \forall\ R_\beta \to \infty \quad \beta \neq \alpha, \\ 0 & \forall\ R_\beta \to 0 \end{cases}$$

and define the difference between Ψ and Φ to be

$$\chi = \Psi - \Phi \ .$$

The function Φ is a known function which is second order differentiable and satisfies the boundary conditions for all reacted configurations of the system. Solve for χ by expanding χ in the asymptotic eigenfunctions of the α channel:

$$\chi = \sum_n f_n^\alpha (R_\alpha)\, \phi_n^\alpha \ .$$

When the expansion representing χ is placed in the Schrödinger equation;

$$(\mathcal{H} - E)\Psi = (\mathcal{H} - E)(\chi + \Phi) = 0 \ ,$$

a coupled inhomogeneous set of differential equations results. Zakhariev proposed that integration of this set of equations would yield functions which solve the reactive collision equations. Section 2 investigates these equations in greater detail. A more complete specification of the formalism proposed by Zakhariev et al is not needed at this time since most applications of this method have not used the minute structure of the M. S. A. equations.

After the complete description of the Method of Subtracted Asymptotics was published, Zakhariev and others used various parts of the formalism in other work. The complete formalism contained in Za67, Ef68a and Ef68b was never used on any system with a well known, theoretically determinable answer.

In his doctoral thesis, Efimenko (Ef68c) used the split solution technique and the Kohn Variational Principle to treat reactions with particle redistribution with variation methods. This material was published in 1970 (Ef70) but the variational formulas were never numerically applied to a reaction.

One numerical calculation which used a large body of the features of M. S. A. was a nucleon-deuteron collision done by Zakhariev, Pustovalov and Efros (Za68a). The major alteration of the formulas used in this reaction was the use of the hyperspherical harmonics as an expansion set for the reaction. The implications of this choice of eigenfunctions will be discussed in section 5. This work was also reported in Za68b and Za69.

Other workers began to select portions of M. S. A. for incorporation into their theoretical treatments as early as 1969. Austern (Au69) used the Method of Subtracted Asymptotics to extend the Sasakawa theory for elastic collisions to reactions. This was a purely formal treatment.

The split solution, variational principle formulas prepared by Efimenko were used by Zakhariev and coworkers (Za70 , Za71) to establish bounds on the probability matrix for reactive encounters.

This work, as were virtually all others using M. S. A., was wholly theoretical in scope.

V. D. Efros contributed to the initial introduction of hyperspherical harmonics into Zakhariev's equations. These functions replaced the asymptotic eigenfunctions originally proposed as an expansion basis for the M. S. A. solution. He further adjusted the founding principles of the original formalism by introducing a variational principle into his later work on nuclear scattering (Ef71 , Zh71).

A final use of the method investigated here was prepared by Kitazoe. Kitazoe (Ki72) created an operator formalism for nuclear reactions which has as its novel point the use of sectional solutions and asymptotic eigenfunctions from each rearrangement channel. His work is thus another formulation of M. S. A.

A review of all of the references that comprise the history of the Method of Subtracted Asymptotics shows that no well posed, simple system which has been solved theoretically has ever been treated by this method. Thus, there has never been an established result which the solution generated by M. S. A. was required to duplicate. The analysis of the method which follows, fills this gap.

The Zakhariev Formulas: A Special Case of a More General Method.

The Method of Subtracted Asymptotics sprang from a synthesis of the basic ideas of subchannel decomposition and Levin's split solution proposal. It is, however, neither a new nor novel method.

The formulas which make up the Method of Subtracted Asymptotics are, for certain special potentials, an application of the technique of eigenfunction expansion. This general method will be discussed briefly at this juncture.

This treatment of eigenfunction expansion techniques for boundary value problems follows that given by Collatz (Co60). A solution Ψ, will be sought to the linear, homogeneous, boundary value problem:

$$L[\Psi] = 0 \text{ in } B, \tag{1a}$$

$$U_i[\Psi] = v_i \quad \text{on } \Gamma \ (i=1 \text{ to } k), \tag{1b}$$

where B is the region which the solution Ψ occupies, Γ is a boundary of the region B, and L and U_i are linear differential expressions which constitute the differential operator and boundary conditions, respectively.

It will be assumed that the boundary conditions,

$$U_i[\Psi] = v_i \text{ on } \Gamma \ (i=1 \text{ to } k), \tag{2}$$

render the solution unique. The problem will first be reduced to one with homogeneous boundary values. Thus, let Φ be a function which satisfies the inhomogeneous boundary conditions of equation 1.2). Also, let Φ possess derivatives of sufficiently high order so that $L[\Phi]$ exists. Then the function

$$u = \Psi - \Phi,$$

satisfies a linear, boundary value problem with homogeneous boundary conditions, namely

$$L[u] = r = L[\Psi] - L[\Phi] = -L[\Phi] \text{ in } B, \tag{3a}$$

$$U_i[u] = 0 \text{ on } \Gamma \quad (i=1 \text{ to } k). \tag{3b}$$

To complete the solution to equation 1.1), assume that the eigenfunction problem equivalent to equation 1.1) possesses a complete system of eigenfunctions $\Lambda_1, \Lambda_2, \ldots$ corresponding to the eigenvalues $\lambda_1, \lambda_2, \ldots$;

$$L[\Lambda_i] = \lambda_i \Lambda_i \quad \text{in} \quad B, \tag{4a}$$

$$U_i[\Lambda_i] = 0 \quad \text{on } \Gamma \, (i=1 \text{ to } k). \tag{4b}$$

Presuming that the function r can be expanded in a uniformly convergent series, define the expansion of r to be

$$r = \sum_{m=1}^{\infty} c_m \Lambda_m. \tag{5}$$

Then, since

$$L[u] = r,$$

the value of u is

$$u = \sum_{m=1}^{\infty} (c_m / \lambda_m) \Lambda_m.$$

The boundary value problem is therefore solved because

$$\Psi = \Phi + u \tag{6a}$$

implies

$$L[\Psi] = L[\Phi] + L[u] = -r + \sum_{m=1}^{\infty} \lambda_m (c_m / \lambda_m) \Lambda_m = \tag{6b}$$

$$-r + r = 0 \quad \text{in } B$$

and

$$U_i[\Psi] = U_i[\Phi] + U_i[u] = v_i + 0 \quad \text{on } \Gamma \ (i=1 \text{ to } k). \tag{6c}$$

A specific application of this general treatment of boundary value problems requires the specification of a region, B; the

boundary, Γ; a differential operator, L; and a set of boundary conditions $U_i[\Psi] = v_i$, (i=1 to k). There must also exist a second order differentiable function Φ which satisfies the boundary conditions of the differential equation and the differential relationship must represent a particular class of eigenvalue problems.

The eigenfunctions for the differential operator must exist in the region B and must form both a distinct spectrum of functions and a complete set. Finally, an application of this formalism is predicated on the ability to expand the inhomogeneity, r, in a uniformly convergent series of eigenfunctions.

Notation Needed to Apply the General Method

For a linear, electronically adiabatic, reactive, three atom collision, Figure 1 presents important notation and the definitions of atom order used in this work. Figure 2 motivates the defi-ition of Γ and B by showing the geometry of the coordinate space in which the reaction occurs. In atom-diatom collisions, the "interaction region" constitutes the zone denoted by B. This definition is displayed graphically in Figure 2. The boundary Γ is choosen to be the two labeled, parallel lines of Figure 2 which bound the interaction region in the reactive channel.

The differential operator for the interaction of three, linearly oriented particles is the Schrödinger operator,

$$L = \mathcal{H} - E.$$

Before further statements can be made about eigenfunction expansions in scattering theory, several definitions must be

established. The term "channel" will be used to denote a particular distribution of the particles of an interaction into widely separated, noninteracting aggregates which are characterized by specific quantum or momentun states.

There are two channels in the collinear collision. They are the entrance channel, denoted AB + C and the reacted channel, denoting an A + BC configuration. The term "subchannel" will refer to one particular distribution of energy into the quantum states and momentum values of the aggregates undergoing collision. Having oscillator AB in state n with atom C possessing momentum k defines one particular subchannel of the entrance channel. See Mo65a for further comments on the definition of channels.

Each subchannel has a definite status in any collision. If the colliding system could exist in some specific subchannel at the total energy given for the collision, then that subchannel is termed open. If it is energetically impossible for the system to exist in a given subchannel, that subchannel is termed closed. Closed subchannels are also called virtuals.

With this terminology established, the process of establishing that the Method of Subtracted Asymptotics is an application of the eigenfunction expansion formalism can continue.

The boundary conditions of this collision are that the total, one entrance subchannel solution for the collision, behaves as a superposition of 1) a unit incoming flux, and, 2) an outgoing

flux scattered into all open entrance subchannels in the entrance channel. In the reacted channel, the solution behaves as an outgoing flux in all open subchannels.

In traveling wave form, the mathematical embodyments of these conditions are:

entrance

$$\Psi_i = \delta_{ij} e^{-ik_i x} + R_{ij} e^{ik_j x} \phi_j(x_{12}), \tag{7a}$$

reacted

$$\Psi_i = \bar{R}_{ij} e^{ik_j x'} \bar{\phi}_j(x_{23}). \tag{7b}$$

In standing wave form, they become

entrance

$$\Psi_i = (\delta_{ij} \sin(k_i x) + R_{ij} \cos(k_j x) \phi_j(x_{12}), \tag{8a}$$

reacted

$$\Psi_i = \bar{R}_{ij} \cos(k_j x') \bar{\phi}(x_{23}). \tag{8b}$$

These equations define the general boundary relations, $U_i[\Psi]$.

Only the boundary condition function, Φ, of the eigenfunction expansion formalism is, as yet, undefined. This function will be specified for the sample cases treated in section 4. With the exception of Φ, all parts of the general formulas of the eigenfunction expansion method have been related to their specific counterparts in the one dimensional scattering equations of the Method of Subtracted Asymptotics.

However, the implications of this part matching between the general formalism and the scattering application of this

formalism show a major flaw in the Method of Subtracted Asymptotics. Efimenko, Zhigunov and Zakhariev proposed that the final solution to the problem, termed u in the general treatment and χ in Ef67b, Za67, Ef68a, and Ef68b, be expanded in eigenfunctions of the diatom, $\phi_j(x_{12})$. The general method of eigenfunction expansions shows that the expansion set must be the set of eigenfunctions determined by the boundary Γ and the region B,

$$(\mathcal{H} - E)\ \Lambda_i(x_{12}) = \lambda_i\ \Lambda_i(x_{12}) \quad \text{in B},$$
$$U_i[\Lambda_i(x_{12})] = 0 \quad \text{on } \Gamma \quad (i=1 \text{ to } k).$$

The diatom eigenfunctions are specified by the region A of Figure 2.

For most systems Zakhariev, Zhigunov and Efimenko proposed to treat with the Method of Subtracted Asymptotics, the expansion in the set $\{\phi_j(x_{12})\}$ will provide a solution which does not cover the region B and, therefore, does not solve the scattering problem. In all cases where the set equality

$$\{\Lambda_i(x_{12})\} = \{\phi_j(x_{12})\}$$

does not hold, the Method of Subtracted Asymptotics, as originally proposed, will give incorrect results for the problem considered.

While the equations prepared by Efimenko, Zhigunov and Zakhariev have never been tested to determine the capacity of M. S. A. to solve the scattering problem, the parent technique of eigenfunction expansion has been tested in several applications

where the solution to a partial differential equation was needed. The text Differential Equations and Applications by Scarborough (Sc65) contains treatments of the equations govering mechanical motion, vibration, support stress and electrical circuits using the eigenfunction expansion technique. The problem of distortion of prisms is solved using eigenfunction expansion in Co60. The same problem is solved using a different technique in Sm65. Finally, in a text by Sobolev (So64), a hyperbolic, partial differential equation is solved using the expansion method.

In section 2, the Method of Subtracted Asymptotics is presented in detail with the correct eigenfunction set for the formalism, the $\{\Lambda_j(x_{12})\}$, used in the formulas. In section 3, various numerical methods for solving the coupled differential equations of the scattering problem are defined and compared. From these numerical techniques, the Gordon method was chosen as the mechanism for solving the differential equation. The application of this method to two potential models in reactive scattering is described in section 4. The conclusions concerning the applicability of the Method of Subtracted Asymptotics are contained in section 5.

2: Detailed Equations for the Method of Subtracted Asymptotics

The Method of Subtracted Asymptotics was posed as a general technique for solving the three-dimensional form of the three particle, Schrödinger equation for energies below that required for the separate existence of the three atoms. The ability of this method to treat arbitrary particle, two-particle oscillator encounters is directly attributable to the formalism's removal of the boundary conditions relating to two of the three possible outcomes of a low energy collision.

$$C + AB \rightarrow C + AB \quad \text{maintained} \qquad (1a)$$

$$C + AB \rightarrow CA + B \quad \text{removed} \qquad (1b)$$

$$C + AB \rightarrow CB + A \quad \text{removed} \qquad (1c)$$

The representation of the Method of Subtracted Asymptotics presented here will not be a general three-dimensional form of the scattering equations. Since the utility of this method was never established, the method was applied to several simple, well investigated, model problems. A great deal of the simplicity of the model collisions treated in section 4 comes from restricting the three colliding particles to a collinear configuration. Figure 3 compares the three dimensional particle configuration to the collinear particle configuration.

All of the equations of this section apply only to a collinear, electronically adiabatic,three-atom collision. These equations are the basis of the computations contained in section 4.

Notation and Terminology:

The asymptotic form of the wavefunction describing a free

particle involved in an interaction is usually posed in traveling wave form:

$$f(x) = Ae^{-ikx} + Be^{+ikx}. \qquad (2)$$

The complex arithmatic of this function can be avoided in numerical computations by using standing waves for all representations of the free particle's wavefunction (Tr70, Gu72a). In standing wave form, equation 2.2) becomes

$$f(x) = A' \sin(kx) + B' \cos(kx). \qquad (3)$$

The coefficients A' and B', of the standing wave are conventionally represented in an R matrix. A definition of the R matrix is contained in Mo65b. A slight change in the notation used for the R matrix will be made in this work to distinguish between matrix elements specific to the reacted channel and those of the entrance channel. Elements of R which describe reacted amplitudes will be denoted $\bar{R}_{ij}$ while inelastic amplitude elements will keep their standard notation of R_{ij}. This distinction will permit a clear formulation of the collision equations.

The coordinates used for these equations are the reduced, mass dependent coordinates previously used in both inelastic and reactive problems (Gu72b, Ta69). The two reduced coordinate sets are

1) Entrance

$$x = (\mu_{12,3}/\mu_{12})^{\frac{1}{2}} [x_3 - (m_1x_1 + m_2x_2)/(m_1 + m_2)] \qquad (4a)$$

$$x_{12} = x_2 - x_1 \qquad (4b)$$

2) Reacted

$$x_{23} = x_3 - x_2 \tag{5a}$$

$$x' = (\mu_{23,1}/\mu_{23})^{\frac{1}{2}} [x_1 - (m_2x_2 + m_3x_3)/(m_2 + m_3)] \tag{5b}$$

where

$$\mu_{ij} = m_i m_j/(m_i + m_j)$$

$$\mu_{ij,k} = m_k(m_i + m_j)/(m_i + m_j + m_k).$$

In these coordinate schemes, the hamiltonian for the reaction can be written in the two forms:

entrance channel

$$\mathcal{H}_e = [\partial^2/\partial x^2 + \partial^2/\partial x_{12}^2 - 2\mu_{12}/\hbar^2 V(x, x_{12})] \tag{6e}$$

reacted channel

$$\mathcal{H}_r = [\partial^2/\partial x'^2 + \partial^2/\partial x_{23}^2 - 2\mu_{23}/\hbar^2 V(x', x_{23})] \tag{6r}$$

In the asymptotic region of the collision, these hamiltonians can be reformulated into a kinetic energy term and the hamiltonian of the two particle oscillator. The oscillator hamiltonians are

entrance channel

$$h_e = (\partial^2/\partial x_{12}^2 - 2\mu_{12}/\hbar^2 V_e(x_{12})) \tag{7e}$$

and reacted channel

$$h_r = (\partial^2/\partial x_{23}^2 - 2\mu_{23}/\hbar^2 V_r(x_{23})) \tag{7r}$$

The operators h_e and h_r define the two sets of eigenfunctions $\{\phi_j(x_{12})\}$ and $\{\bar{\phi}_k(x_{23})\}$ by the relations:

entrance channel

$$\{\partial^2/\partial x_{12}^2 - 2\mu_{12}/\hbar^2 (V_e(x_{12}) - \epsilon_j)\} \phi_j(x_{12}) = 0 \tag{8e}$$

and reacted channel

$$\left\{ \partial^2/\partial x_{23}^2 - 2\mu_{23}/\hbar^2 \left(V_r(x_{23}) - \epsilon_k \right) \right\} \bar{\phi}_k(x_{23}) = 0 \qquad (8r)$$

The asymptotic region will be defined as that zone of the potential surface for which

$$V(x, x_{12}) = V(x_{12}) \qquad (9e)$$

or

$$V(x', x_{23}) = V(x_{23}). \qquad (9r)$$

An alternative statement of the definition of the asymptotic region which is very useful in defining the boundary Γ, is that the asymptotic region is that zone of the potential surface within which the lines connecting points of equal potential (equipotential lines) are perpendicular to the oscillator's coordinate, x_{12} or x_{23}. The term interaction region will apply to all areas that are not asymptotic.

In all discussions of the formalism of the Method of Subtracted Asymptotics, the notation for the number of subchannels used in any decomposition will be:

P = the number of open entrance subchannels,

Q = the number of open reacted subchannels,

W = the number of total entrance subchannels used in an expansion.

The Formalism.

The problem to be solved in the interaction region, the domain B for scattering, can be expressed as

$$(\mathcal{H} - E)\Psi_n = 0 \quad \text{in B}, \qquad (10a)$$

$$U_i[\Psi_n] = \Psi_{in} = \bar{\phi}_i(x_{23})\bar{R}_{in}\cos(k_i x') \text{ on } \Gamma = x^{\circ\prime}, \ (i=1 \text{ to } Q), \quad (10b)$$

$$\Psi_{in} = \phi_i(x_{12})(\delta_{in}\sin(k_i x) + R_{in}\cos(k_i x)), \ (i=1 \text{ to } P) \text{ on } x^{\circ}. \quad (10c)$$

The two points x° and $x^{\circ\prime}$ denote the start of the asymptotic region in the entrance and reacted channels, respectively. The value $x^{\circ\prime}$ defines the line Γ needed in the Method of Subtracted Asymptotics.

This general statement of the scattering problem is not as complete as possible. In time independent scattering theory, which equation 2.10) represents, the energy E is taken as a fixed parameter of the system. Fixing E allows all energetically accessible states of the system to be populated.

This implies that the target diatom is not restricted to be in state n as the unscattered beam of incoming atoms moves towards it. The target can instead, be in an array of states j = 1 to P, limited only by the inequality $\epsilon_p \leq E$.

Thus, there are P solutions to equations 2.10), each characterized and distinguishable by the fact that the unit incoming flux of free atoms is impacting on the diatom while that oscillator is in a particular state, j = 1 to P.

In later portions of this study, the fact that there exists P solutions to this problem must be taken into account. Initially, however, only one representative solution, Ψ_n, of the set of solutions $\{\Psi_j\}$ will be used in the discussion of reactive encounters.

The single solution Ψ_n, will be obtained by using the eigenfunction expansion technique. The first step in this technique is

to choose a function that will make the boundary conditions on Γ homogeneous. The boundary condition function, Φ_n, must be second order differentiable and must span the interaction region.

The general conditions on Φ_n are

$$\lim_{x' \to 0} \Phi_n = 0 \tag{11a}$$

and

$$\lim_{x' \to x^{\circ\prime}} \Phi_n = \sum_{j=1}^{Q} \bar{R}_{jn} \bar{\phi}_j(x_{23}) \cos(k_j x'). \tag{11b}$$

These conditions have been met by preparing a function Φ'_n in the form

$$\Phi'_n = \sum_{i=1}^{M} \sum_{j=1}^{Q} x'^{\,i} D^i_{jn} \bar{\Lambda}_j(x_{23})\, g_i(x'). \tag{12}$$

The integer M defines the degree of expansion of Φ_n in an independent function set. The functions $\{\bar{\Lambda}_j(x_{23})\}$ are the eigenfunctions of the interaction region prepared by imposing zero boundary conditions at $x_{23} = 0$ and $x = x^\circ$. The functions $\{g_i(x')\}$ are a linearly independent set of functions of x' which span the region from $x' = 0$ to $x' = \Gamma = x^{\circ\prime}$.

It is important to note that Φ_n, as shown in equation 2.11b), is dependent on the unknowns $\{\bar{R}_{jn}\}$. Thus, the expansion of equation 2.12) matches only the <u>functional</u> nature of the complete function Φ_n. By multiplying Φ'_n by the $\bar{R}$ matrix elements $\{\bar{R}_{jn}\}$, Φ_n is formed as shown in equation 2.11b).

This specification of Φ_n by its satisfaction of the two conditions of equation 2.11) can be posed in an alternative form. Let Φ_n be defined for all x_{23} such that

$$\Phi_n(x', x_{23}) = 0 \quad \text{for } x_{23} > x^\circ,$$

yet Φ_n satisfies equation 2.11). Then for $x' > x^{\circ\prime}$, take Φ_n to be the asymptotic form of Ψ_n, which equation 2.11b) says it must be at $\Gamma = x^{\circ\prime}$. However, Φ_n must go to zero at $x' = 0$ and $x_{23} = 0$, and contains the unknowns $\{\bar{R}_{jn}\}$.

Hence, match the functional part of Φ_n, $\bar{\phi}_j(x_{23})\cos(k_j x')$, to a set of functions of the form

$$\Phi'_{jn} = x' D^i_{jn} \bar{\Lambda}_j(x_{23}) g_i(x') \quad \text{at } \Gamma,$$

so that a continuous function is formed for all x'. Multiplying this "continuation function", Φ'_n, by $\underset{\sim}{\bar{R}}$ gives the Φ_n needed to solve the boundary condition of equation 2.10b).

Completing the definition of Φ_n is now a matter of preparing the eigenfunctions $\{\bar{\Lambda}_i(x_{23})\}$, which are dictated by the potential surface, $V(x', x_{23})$; choosing the expansion set $\{g_j(x')\}$; and calculating the matching condition constants D^i_{jn}. As will be seen later, the final step of calculating the D^i_{jn} occurs in the analysis of the total wavefunction.

The boundary condition function Φ_n, is dependent on two sets of unknown constants, $\{\bar{R}_{jn}\}$ and $\{D^i_{jn}\}$. But, since the Schrödinger equation contains a linear operator, $(\mathcal{H} - E)$, these constant unknowns of Φ_n will not be affected by any manipulations of the differential equation. Therefore, Φ_n will be assumed to satisfy the boundary condition of equation 2.10b) via its unknown constants and the expansion in eigenfunctions will be undertaken.

A general solution

$$\Psi_n = \Phi_n + \chi_n \tag{13}$$

is being sought for the Schrödinger equation. The function Φ_n has satisfied the reacted boundary condition at Γ so that χ_n is the solution to the inhomogeneous, inelastic problem

$$(\mathcal{H} - E)\chi_n = -(\mathcal{H} - E)\Phi_n \quad \text{in B,} \tag{14a}$$

$$\chi_{in} = \phi_i(x_{12})(\delta_{in}\sin(k_i x) + R_{in}\cos(k_i x)) \quad (i=1 \text{ to } P), \tag{14b}$$

$$U_i(\chi_n) = \chi_{in}(x', x_{23}) = 0 \text{ on } \Gamma = x^{\circ\prime}. \tag{14c}$$

The inhomogeneity of equation 2.14a) arises naturally

$$\begin{aligned}(\mathcal{H}-E)(\Psi_n) &= (\mathcal{H}-E)(\Phi_n + \chi_n) = 0 \\ &\rightarrow (\mathcal{H}-E)\chi_n = -(\mathcal{H}-E)\Phi_n,\end{aligned} \tag{15}$$

from the requirement that $\Phi_n(x', x_{23})$ satisfy only the boundary condition at Γ. The function $\Phi_n(x', x_{23})$ does not satisfy the differential equation.

The major thesis of the method of eigenfunction expansions can now be brought to bear on the solution of the χ_n relation, equation 2.14). The desired function, χ_n, will be found in terms of the eigenfunctions, $\Lambda_j(x_{12})$, which span the domain B in the direction x_{12}. This eigenfunction set is defined by the equation,

$$\left\{\partial^2/\partial x_{12}^2 - 2\mu_{12}/\hbar^2\,(V^\circ(x, x_{12}) - \epsilon_j)\right\}\Lambda_j(x_{12}) = 0. \tag{16}$$

Equation 2.16) contains the full interaction region potential, $V(x, x_{12})$. Since $V(x, x_{12})$ will in general vary along the x coordinate, the eigenfunction set $\{\Lambda_j(x_{12})\}$ will, in general, be functions of the coordinate x also.

The additional coordinate dependence of $\{\Lambda_j(x_{12})\}$ has been suppressed in the notation for the eigenfunction set. However, the practical implications of the variation of the $\{\Lambda_j(x_{12})\}$ are not suppressible and these effects significantly alter the mathematical techniques used to solve the χ_n equation.

The variation of the eigenfunction set $\{\Lambda_j(x_{12})\}$ with x mandates that χ_n be composed of expansions in a series of different eigenfunction sets, $\{\Lambda_j(x_{12})\}^m$. Each of these eigenfunction spectrums solves equation 2.16) for a small domain of the x variable,

$$a \leq x \leq b.$$

To continue the expansion solution, χ_n, beyond this region, $[a, b]$, a new set of eigenfunctions satisfing equation 2.16) for the potential

$$V^1(x, x_{12}) \ni b \leq x \leq c,$$

must be created. The propagation of χ_n over small regions of the x coordinate must be continued for the entire interaction region.

The Eigenfunction Expansion

Only the specification of an exact potential surface, $V(x, x_{12})$, in equation 2.16) obstructs a complete evaluation of the eigenfunctions $\{\Lambda_j(x_{12})\}$. The $\{\Lambda_j(x_{12})\}$ of whatever $V(x, x_{12})$ is chosen for the problem will be used to expand $\chi_n(x, x_{12})$ into an eigenfunction series,

$$\chi_n(x, x_{12}) = \sum_{j=1}^{W} f_{jn}(x)\Lambda_j(x_{12}). \qquad (17)$$

Place the expansion of equation 2.17) into equation 2.15).

$$(\mathcal{H}-E)\sum_{j=1}^{W} f_{jn}(x)\Lambda_j(x_{12}) = -(\mathcal{H}-E)\Phi_n \tag{18a}$$

or

$$\left\{\partial^2/\partial x^2 + \partial^2/\partial x_{12}^2 - 2\mu_{12}/\hbar^2 (V(x,x_{12}) - E)\right\}\sum_{j=1}^{W} f_{jn}(x)\Lambda_j(x_{12}) = -(\mathcal{H}-E)\Phi_n \tag{18b}$$

Add and subtract the function

$$-2\mu_{12}/\hbar^2 (V^\circ(x,x_{12}) - \epsilon_j)$$

from equation 2.18) and project the resulting formula on the set $\{\Lambda_p(x_{12})\}$ for fixed x to obtain

$$\left\{\partial^2 f_{pn}(x)/\partial x^2 - 2\mu_{12}/\hbar^2 \sum_{j=1}^{W} \int_0^\Gamma \Lambda_p(x_{12})(V(x,x_{12}) - V^\circ(x,x_{12}) - E + \epsilon_j)\Lambda_j(x_{12})\,dx_{12}\, f_{jn}(x)\right\} = -\int_0^\Gamma \Lambda_p(x_{12})(\mathcal{H}-E)\Phi_n(x',x_{23})\,dx_{12},$$

for p=1 to W. (19a)

Equation 2.19a) plus the boundary conditions

$$\chi_{in} = \phi_i(x_{12})(\delta_{in}\sin(k_n x) + R_{in}\cos(k_i x)) \text{ on } x^\circ,\ \chi_{in}(0) = 0 \tag{19b}$$

completely determine the expansion coeffecients $\{f_{jn}(x)\}$. In later equations, the notation

$$V_{pj}(x) = \int_0^\Gamma \Lambda_p(x_{12})(V(x,x_{12}) - V^\circ(x,x_{12}) - E + \epsilon_j)\Lambda_j(x_{12})\,dx_{12}$$

will be used to represent the integrals containing the potential function.

The solutions to equation 2.19) will be obtained by one of the several numerical techniques discussed in section 3. The basic theory of solution combination that permits the numerical techniques to seek wavefunctions with arbitary boundary behavior

at x° will be presented at this point since it controls the structure of the analysis equations.

The Principle of Superposition

An ordinary, linear, differential equation of order n has n linearly independent solutions from which any solution to the equation can be prepared. This is not true for a partial differential equation. For the linear partial differential equation, only the Principle of Superposition holds.

The Principle of Superposition allows the solution to a linear partial differential equation containing N separate, non-homogeneous restrictions (differential relations and boundary conditions) to be solved by a set of N separate solutions to a lesser problem. Each function of the set of N solution functions is of a form such that each distinct solution satisfies one distinct inhomogeneous condition out of N such conditions and also satisfies the homogeneous form of the other N - 1 conditions. The total solution is then the sum of these particular N solutions (We-65a).

The Superposition Principle allows the full solution to equation 2.19) to be broken up into homogeneous terms and inhomogeneous terms. Because of this separation, equation 2.17) can be rewritten as

$$\chi_n(x, x_{12}) = \sum_{j=1}^{W} (f_{jn}^h(x) + f_j^I(x)) \Lambda_j(x_{12}). \qquad (20)$$

Here, the inhomogeneous function $f_j^I(x)$ solves one portion

of equation 2.19). The homogeneous function, $f^{h}_{jn}(x)$, solves the homogeneous form of equation 2.19a), namely:

$$\left\{ \partial^2 f^{h}_{pn}(x)/\partial x^2 - 2\mu_{12}/\hbar^2 \sum_{j=1}^{W} V_{pj}(x) f^{h}_{jn}(x) \right\} = 0 \ (p=1 \text{ to } W), \tag{21a}$$

$$\chi_{in}(x, x_{12}) = \phi_i(x_{12})(\delta_{in}\sin(k_n x) + R_{in}\cos(k_i x)). \text{ at } x = x^{\circ} \tag{21b}$$

The homogeneous and inhomogeneous parts of the expansion for $\chi_n(x, x_{12})$ are manipulated differently during the construction of the total wavefunction. Hence, the logic and formalism for creating these two solution types will be expounded separately so that the methods involved in forming $f^{h}_{jn}(x)$ and $f^{I}_{j}(x)$ are made clear.

The Homogeneous Solution

The homogeneous solution to the inelastic scattering problem represented by equation 2.21) is obtained by superposition of linearly independent solution vectors. These solution vectors solve equation 2.21a) but do not solve equation 2.21b).

The entire collection of W functions $\{ f^{h}_{jn}(x), j = 1 \text{ to } W \}$ constitutes one solution vector. For most inelastic scattering problems (Ba65, Di68a, Go69), a total of W such solution vectors are prepared in such a manner that the wronskian of these W solutions is not zero at any point within B, the interaction region. A non-vanishing wronskian for the W groups, $\{ \{ f^{h}_{jn}(x), j = 1 \text{ to } W \}; n = 1 \text{ to } W \}$, is achieved by replacing the boundary conditions of equation 2.21b) by a set of linearly independent boundary conditions. The independent boundary

conditions permit the numerical method being used to generate linearly independent solutions.

The Inhomogeneous Solution

The inhomogeneous solution to equation 2.19) is also a sum of separate solution terms. The creation of the inhomogeneous solution is a straightfoward application of the Principle of Superposition.

The inhomogenaity of equation 2.19a) is a sum of separate integrals of the form

$$-\int_0^{\Gamma} \Lambda_p(x_{12})(\mathcal{H}-E)\Phi_n(x', x_{23})\,dx_{12} = -\sum_{l=1}^{Q}\sum_{k=1}^{M} \int_0^{\Gamma} \Lambda_p(x_{12})(\mathcal{H}-E)x' D_{ln}^k \bar{\Lambda}_l(x_{23})\, g_k(x')\,dx_{12}. \tag{22}$$

The Superposition Principle states that a particular solution to the total inhomogeneous equation is a sum of functions, each one of which solves a single term inhomogeneous equation of the type

$$D_{ln}^k\left\{ {}^{\partial^2 f^I_{pkl}(x)}/_{\partial x^2} - {}^{2\mu_{12}}/_{\hbar^2} \sum_{j=1}^{W} V_{pj}(x) f^I_{jkl}(x)\right\} = -D_{ln}^k \int_0^{\Gamma} \Lambda_p(x_{12})(\mathcal{H}-E)x' \bar{\Lambda}_l(x_{23})\, g_k(x')\,dx_{12}. \tag{23}$$

One solution vector for the inhomogeneous equation is, therefore,

$$\{f^I_j(x)\} = \sum_{l=1}^{Q}\sum_{k=1}^{M} f^I_{jkl}(x). \tag{24}$$

Presuming that some numerical technique has been applied to the homogeneous and inhomogeneous equations and the prescribed solutions have been generated, a set of W + 1 solution vectors are now at hand to solve the inelastic scattering problem

of equation 2.19). These solution vectors are the W homogeneous solutions $\{\{f_{jk}^{h}(x), j = 1 \text{ to } W\}; k = 1 \text{ to } W\}$ and the one particular inhomogeneous solution, $\{f_{j}^{I}(x), j = 1 \text{ to } W\}$.

Before further manipulations of this solution set are made, the significance of the "solution vectors" will be specified so that the precise meaning of the constructs being used in these equations will not be lost. A solution vector, as an ordered sequence of functions in one variable, is a convenient representation for one solution to a two variable partial differential equation. The solution vector is composed of the expansion coefficients of an eigenfunction series representation of one solution to the differential equation,

$$\chi(x, x_{12}) = \sum_{j=1}^{W} F_j(x)\, \phi_j(x_{12}).$$

The fact that the F_j's satisfy a differential equation or are functions of the variable x is important only in calculating these terms. The set of W expansion coefficients called a solution vector above, can also be looked on as a state vector in Hilbert space (Be68). This view is, however, the most obtuse vantage point available for discerning the role of the $F_j(x)$ set as expansion coefficients.

The Method of Weighted Residuals

The W + 1 solutions will be combined to create the single set of eigenfunction expansion coefficients shown in equation 2.17) by using equation 2.20). Because of the methods used to con-

struct the W + 1 solution vectors, the function:

$$\sum_{j=1}^{W} (f_j^I(x) + \sum_{k=1}^{W} c_k f_{jk}^h(x)) \Lambda_j(x_{12}) \qquad (25)$$

solves equation 2.19a) and the constants c_k are available to meet the boundary conditions of equation 2.19b). This process of solution recombination is a well established technique for solving partial differential equations. The procedure of developing a solution of the partial differential equation from a constant coefficient series of independent solutions to that equation is sometimes termed the Method of Weighted Residuals (Fi72a). This method has been applied in virtually every area of science in which partial differential equations are encountered.

The techniques for insuring minimization of the expansion constants, such as the Trefftz method (Co60b), are seldom applied to the scattering equations. Instead, matrix matching equations have heretofore been used to obtain the set of c's. These matrix methods constitute the analysis equations.

The Analysis:

Two separate approaches to the problem of obtaining the elements of the R matrix from the Method of Subtracted Asymptotics' solution have been investigated. The first analysis technique was suggested by Zakhariev in the original publications on M. S. A. (Ef68a, Ef68b). The second technique was developed to overcome the restrictions of the first analysis method.

The first analysis method can be presented only after a compact notation is defined for the components of the two parts

of the wavefunction, $\Phi_n(x', x_{23})$ and $\chi_n(x, x_{12})$. The definitions will start with the components of $\Phi_n(x', x_{23})$ within the interaction region.

Here, from equations 2.11b) and 2.12), the form of Φ_n is

$$\Phi_n(x', x_{23}) = \sum_{j=1}^{Q} \sum_{i=1}^{M} \bar{R}_{jn} x' D_{jn}^{i} \Lambda_j(x_{23}) g_i(x').$$

Define the vector $\vec{\vec{R}}_n$ as that sequence of elements such that

$$\vec{\vec{R}}_{jn} = \bar{R}_{jn}, \qquad j = 1 \text{ to } Q.$$

The matrix $\underset{\sim}{D}^{i}$ will be such that

$$\underset{\sim}{D}^{i}_{jn} = D^{i}_{jn}, \qquad j = 1 \text{ to } Q,$$

while the vector of eigenfunctions for the reacted channel at Γ will be $\vec{\vec{\Lambda}}$,

$$\vec{\vec{\Lambda}}_j = \bar{\Lambda}_j(x_{23}). \qquad j = 1 \text{ to } Q.$$

The functions $g_i(x')$ will be gathered into a matrix, $\underset{\sim}{G}$, so that

$$\underset{\sim}{G}_{ij} = g_i(x')\delta_{ij}, \qquad i = 1 \text{ to } M.$$

The value of $\Phi_n(x', x_{23})$ then becomes

$$\Phi_n(x', x_{23}) = x' \vec{\vec{R}}_n \underset{\sim}{D}^{i} \vec{\vec{\Lambda}} \underset{\sim}{G}. \qquad (26)$$

For the entrance channel, χ_n will have several vector components also. The homogeneous solution vectors $\{\{f^{h}_{jn}(x), j = 1 \text{ to } W\}; n = 1 \text{ to } W\}$ will be lumped into a matrix, $\underset{\sim}{F}^{h}$, so that

$$\underset{\sim}{F}^{h}_{jn} = f^{h}_{jn}(x), \qquad j = 1 \text{ to } W.$$

The particular solution of the inhomogeneous equation can also be expressed as a matrix, F^{Ii}, with the definition

$$\underset{\sim}{F}^{Ii}_{jk} = f^{I}_{jki}(x) \qquad (27)$$
$$j=1 \text{ to } W,\ k=1 \text{ to } \Omega,\ i=1 \text{ to } M,$$

where j is the subchannel eigenfunction index for the entrance channel, k is the eigenfunction index for the reacted channel and i is the index of the expansion function in Φ_n to which this solution corresponds. As equation 2.27) implies, the particular inhomogeneous solution is independent of the total solution index, n. The constants which multiply $\underset{\sim}{F}^{Ii}$ introduce a dependence on n in the inhomogeneity.

The set of combination constants called for by equation 2.25) will be grouped together as a vector, $\vec{C}_n$,

$$\vec{C}_n = c_{in} \qquad i = 1 \text{ to } W,$$

and the eigenfunctions of the interaction region will compose the vector $\vec{\Lambda}$,

$$\vec{\Lambda}_j = \Lambda_j(x_{12}), \qquad j = 1 \text{ to } W. \qquad (28)$$

The full solution to equation 2.19) becomes

$$\vec{X}_n = \vec{\Lambda}\left\{ \underset{\sim}{F}^{h}\vec{C}_n + \sum_{i=1}^{M} \underset{\sim}{F}^{Ii}\,\underset{\sim}{D}^{i}\,\vec{\vec{R}}_n \right\}$$

in this notation.

The boundary conditions of equation 2.19b) and 2.11b) will also be posed in vector form. The elements of the R matrix in the entrance channel form the vector $\vec{R}_n$,

$$\vec{R}_{jn} = R_{jn}.$$

The two sets of asymptotic eigenfunctions, $\phi_j(x_{12})$ and $\bar{\phi}_j(x_{23})$, form the two vectors

$$\vec{\phi}_j = \phi_j(x_{12})$$

and

$$\vec{\bar{\phi}}_j = \bar{\phi}_j(x_{23}),$$

valid in the entrance and reacted channel asymptotic regions, respectively. Also needed to represent the asymptotic wave-function, Ψ_n, are the diagonal matrices of standing waves,

$$\underset{\sim}{S}_{jk}(x) = \sin(k_j x)\delta_{jk} \tag{29a}$$

$$\underset{\sim}{C}_{jk}(x) = \cos(k_j x)\delta_{jk} \tag{29b}$$

and

$$\underset{\sim}{C}_{jk}(x') = \cos(k_j x')\delta_{jk}. \tag{29c}$$

Equations 2.29b) and 2.29c) are not ment to imply that k_j(entrance channel) = k_j(reacted channel) though this may occur in some cases of the scattering problem. The definition of the wave vector, k_j, at any point is

$$k_j = \left[{}^{2\mu_{12}}/_{\hbar^2} (E - \epsilon_j - V(x, x_{12}) + V^\circ(x, x_{12})) \right]^{\frac{1}{2}}$$

or

$$k_j = \left[{}^{2\mu_{23}}/_{\hbar^2} (E - \epsilon_j - V(x', x_{23}) + V^\circ(x', x_{23})) \right]^{\frac{1}{2}},$$

with the $j^{\underline{th}}$ eigenvalue of the entrance or reacted channel set of eigenvalues represented by ϵ_j.

The boundary conditions of the scattering solution are expressible as

$$\Psi_n(x, x_{12}) = \vec{\phi}(x_{12}) \left\{ \underset{\sim}{S}(x)\vec{\delta}^n + \underset{\sim}{C}(x)\vec{R}_n \right\} \quad \text{at } x = x^\circ \tag{30a}$$

and

$$\Psi_n(x', x_{23}) = \vec{\bar{\phi}}(x_{23})\, \underset{\sim}{C}(x')\vec{\bar{R}}_n \quad \text{at } x' = x^{\circ\prime}. \tag{30b}$$

The vector $\vec{\delta}^n$ is a vector of P elements, only one of which is

non-zero. The single non-zero element is a Kronecker delta function,

$$\vec{\delta}^{n}_{n} = \delta_{nn}.$$

The total wavefunction Ψ_n representing a unit flux, incoming amplitude in entrance subchannel n, must be expressible as

$$\Psi_n = \Phi_n + \chi_n. \tag{31}$$

For Ψ_n to be continuous over the entire path of the reaction, the representations of equations 2.30) and 2.31) must match at the two lines $x = x^\circ$ and $x' = x^{\circ\prime}$.

Zakhariev proposes that this condition be met by a term by term matching of the two functional relations established by setting $\Phi_n(x', x_{23}) + \chi_n(x, x_{12})$ equal to the representations of equation 2.30) at the appropriate lines. This implies

$$\Phi_n(x', x_{23}) + \chi_n(x, x_{12}) = \vec{\phi}(x_{12})\{\underset{\sim}{S}(x)\vec{\delta}^{n} + \underset{\sim}{C}(x)\vec{R}_n\} \quad \text{at } x = x^\circ \tag{32a}$$

and

$$\Phi_n(x', x_{23}) + \chi_n(x, x_{12}) = \vec{\vec{\phi}}(x_{23})\underset{\sim}{C}(x')\vec{\vec{R}}_n \quad \text{at } x' = x^{\circ\prime}. \tag{32b}$$

The term by term matching of the functions at the interaction region boundary is achieved by creating the W distinct equations made by multiplying equation 2.32a) by each element of $\vec{\phi}$ and the Q distinct equations made by multiplying equation 2.32b) by one element of $\vec{\vec{\phi}}$, then integrating the equations on x_{12} or x_{23}, respectively.

Generally, the number of unknowns contained in equation 2.32) will exceed the number of equations generated by term by term matching. Zakhariev suggested that the unitarity condition

which the R matrix satisfies be imposed as additional restraints in the analysis to complete the set of analysis equations. These unitarity conditions are

$$\sum_{j=1}^{P} k_j/k_n R_{jn}^2 + \sum_{j=1}^{Q} k_j/k_n \bar{R}_{jn}^2 = 1, \quad n = 1 \text{ to } P. \tag{33}$$

The unitarity conditions and the term by term matching conditions provide one possible set of analysis equations. Another system of analysis equations can be prepared by the expansion of the interaction region solution at the regional boundaries.

This second method, the expansion technique for creating a set of analysis equations, has been used in several studies of the quantum scattering equations (Di68, Ba65, Le68a). The basic concept of this approach to scattering analysis is that all parts of the solution created in the interaction region are to be represented in a function expansion of the form

$$\phi(x_{12})\{\underset{\sim}{S}(x)\underset{\sim}{A} + \underset{\sim}{C}(x)\underset{\sim}{B}\} \tag{34}$$

at the boundary $x = x^\circ$. The matrices $\underset{\sim}{A}$ and $\underset{\sim}{B}$ contain constants.

The expression of the total interaction region solution in the form of equation 2.34) is accomplished by expanding each part of the solution in a distinct series. Thus, at $x = x^\circ$,

$$\Phi_n(x', x_{23}) + \chi_n(x, x_{12}) = x' \vec{\Lambda} \vec{\bar{R}}_n \underset{\sim}{D}^i \underset{\sim}{G} + \vec{\Lambda}\{\underset{\sim}{F}^h \vec{C}_n + \sum_{i=1}^{M} F^{Ii} \underset{\sim}{D}^i \vec{\bar{R}}_n\}.$$

Hence, if

$$x'\vec{\Lambda}\,\underset{\sim}{G} = \vec{\phi}(x_{12})\{\underset{\sim}{S}(x)\underset{\sim}{A}_p + \underset{\sim}{C}(x)\underset{\sim}{B}_p\}, \tag{35a}$$

$$\vec{\Lambda}\,\underset{\sim}{F}^h = \vec{\phi}(x_{12})\{\underset{\sim}{S}(x)\underset{\sim}{A}_h + \underset{\sim}{C}(x)\underset{\sim}{B}_h\} \tag{35b}$$

and

$$\vec{\Lambda}\underset{\sim}{F}^{Ii} = \vec{\phi}(x_{12})\{\underset{\sim}{S}(x)\ \underset{\sim}{A}_I^i + \underset{\sim}{C}(x)\underset{\sim}{B}_I^i\}, \qquad \text{for } (i = 1 \text{ to } M) \tag{35c}$$

then, by the definition of Ψ_n at $x = x^\circ$,

$$\vec{\phi}(x_{12})\{\underset{\sim}{S}(x)\vec{\delta^n} + \underset{\sim}{C}(x)\vec{R}_n\} = \vec{\phi}(x_{12})\{\underset{\sim}{S}(x)[\underset{\sim}{A}_p\vec{\vec{R}}_n\underset{\sim}{D}^i + \underset{\sim}{A}_h\vec{C}_n + \sum_{i=1}^{M}\underset{\sim}{A}_I^i\underset{\sim}{D}^i\vec{\vec{R}}_n] + \underset{\sim}{C}(x)[\underset{\sim}{B}_p\vec{\vec{R}}_n\underset{\sim}{D}^i + \underset{\sim}{B}_h\vec{C}_n + \sum_{i=1}^{M}\underset{\sim}{B}_I^i\underset{\sim}{D}^i\vec{\vec{R}}_n]\}. \tag{36}$$

By the linear independence of the two standing wave components of this equation, $\underset{\sim}{S}(x)$ and $\underset{\sim}{C}(x)$, it must occur that

$$\vec{\delta^n} = \underset{\sim}{A}_p\vec{\vec{R}}_n\underset{\sim}{D}^i + \underset{\sim}{A}_h\vec{C}_n + \sum_{i=1}^{M}\underset{\sim}{A}_I^i\underset{\sim}{D}^i\vec{\vec{R}}_n \tag{37a}$$

and

$$\vec{R}_n = \underset{\sim}{B}_p\vec{\vec{R}}_n\underset{\sim}{D}^i + \underset{\sim}{B}_h\vec{C}_n + \sum_{i=1}^{M}\underset{\sim}{B}_I^i\underset{\sim}{D}^i\vec{\vec{R}}_n. \tag{37b}$$

Equation 2.37) must be solved in conjunction with the continuity condition at Γ:

$$\Phi_n(x', x_{23}) = \vec{\vec{\phi}}\,\underset{\sim}{C}(x')\vec{\vec{R}}_n = \Psi_n(x', x_{23}) \text{ on } \Gamma, \tag{38}$$

to obtain values for the unknowns $\vec{C}_n$, $\underset{\sim}{D}^i$ for i=1 to M, $\vec{\vec{R}}_n$ and $\vec{R}_n$. The values determined with equations 2.37) and 2.38) represent the simplest approximation to the true solution to the differential equation. Generalized least squares (Fi72b) or Trefftz condition (Tr26, Tr28) analysis could also be used to obtain a better approximation to the vector $\vec{C}_n$ and, consequently, a better approximation to the other unknowns. However, numerical stability problems preclude the use of these approaches to the exact solution.

Equations 2.37) and 2.38) constitute a complete set of analysis equations. There is no need to impose time reversability or unitarity constraints on the $\underset{\sim}{R}$ matrix under this form of analysis. Further, as will be detailed in section 4, Zakariev's proposal for solution analysis restricts the number of subchannels that can be used in developing the solution, χ_n. Since χ_n is an eigenfunction expansion solution, this is a very serious limitation on the solution of the partial differential equation. No such restriction on the number of eigenfunction terms which may enter into $\chi_n(x, x_{12})$ through equation 2.17) arises in the second analysis technique.

The analysis equations complete the formulas of the Method of Subtracted Asymptotics and add the final elements to the formalism for applying the technique of eigenfunction expansion to scattering problems. The numerical capabilities of this system have been tested and the results of these tests are contained in the following sections of this work.

3: Numerical Techniques for the Solution of Coupled Ordinary Differential Equations

The Method of Subtracted Asymptotics reduced the solution of the Schrödinger equation, equation 2.10), to a set of coupled, ordinary differential equations with two point boundary conditions, as shown in equation 2.19). These coupled equations must still be solved by some numerical technique. The choice of this numerical method is not dictated by the formulas of section 2 but can be chosen on the basis of speed and accuracy in solving coupled differential equations.

The mechanisms for solving an equation set similar to equation 2.19) divide roughly into two groups. The groups are differentiated by the types of boundary condition data they will accept. Those numerical techniques which use the value and the derivatives of the desired solution at one point to determine the total solution will be termed Cauchy techniques. The second group of numerical methods require the value of the total solution at several points or lines of the boundary of the region considered. This second group of methods may also create a solution for which only a derivative of the solution at several points or lines is known. These methods are termed Dirichlet techniques when solution values are known and Neumann techniques when solution derivatives constitute the boundary data.

The first group of numerical formulas, Cauchy Data techniques, are usually used to solve hyperbolic or parabolic differential

equations. Elliptic differential equations, such as the Schrödinger equation, with Cauchy boundary value data are termed not "properly posed", a definition first used by Hadamard (Ha23). Cauchy boundary data do not restrict the solution to an elliptic partial differential equation so that slight changes in the boundary conditions cause slight changes in the solution (We65). Thus, Cauchy methods have a tendency to diverge when used to solve scattering problems. This behavior mandates that stabilizing transforms be introduced into any Cauchy method applied to an elliptic system.

An elliptic partial differential equation with Dirichlet or Neumann boundary value data represents a "properly posed" problem. Further, scattering problems virtually always have their boundary value data in Dirichlet form. For this reason, Neumann data, which is a knowledge of the solution's derivative at several points or lines, will not be considered in this section.

Dirichlet methods are the standard methods for solving ordinary, coupled, differential equations from an elliptic partial differential equation. These numerical regimes are both very stable and very extensively investigated.

In each of the two classes of numerical methods, there are a multitude of techniques which could be applied to the problem of equation 2.19). Thinning this polyglot of methods down to a few particularly useful formalisms is easy if equation 2.19) is taken to be an inelastic scattering problem. Numerical methods

for inelastic scattering constitute a small subset of each of the two classes of boundary value methods considered here. The viable Cauchy techniques will be treated first, followed by a short investigation of useful Dirichlet techniques.

As these numerical methods are discussed, it will initially be assumed that the system of equations being solved is homogeneous. Consideration will be given to any adjustments that must be made to each numerical method to enable it to treat an inhomogeneous equation set in a separate portion of the discussion of the techniques of each boundary condition class.

Cauchy Methods:

One of the first studies of the quantum, inelastic scattering of atoms was performed using a method termed DRILL (Ri68). DRILL uses a simple predictor-corrector integration formula such as the Adams-Moulton or Milne equations (Ca69), with periodic transformations of the solution to remove any instabilities that may develop in the solution matrix.

This method has been superceded by two other techniques and is mentioned here predominately for its historical significance.

In 1968, Lester and Bernstein (Le68a) published an application to the rotational scattering problem of an integration technique developed by Rene de Vogelaere (Vo55). This mode of solving the coupled, ordinary equations of the scattering problem makes specific use of the absence of a first derivative term in equation 2.19). Such specific optimization of the integration method

makes the de Vogelaere formulas a very efficient means of solving the scattering equations (Na61 , Le68c).

If the coupled relationships of equation 2.19) are rewritten as

$$\partial^2 f_{in}(x)/\partial x^2 = F_i(x; f_{1n}(x), f_{2n}(x), \ldots, f_{wn}(x)), \quad i = 1 \text{ to } W, \quad (1)$$

and a third index is added to all functions such that

$$f_{in,j}(x) = f_{in}(x_0 + jh), \quad (2a)$$

$$F_{i,j} = F_i(x_0 + jh; f_{1n,j}(x), f_{2n,j}(x), \ldots, f_{wn,j}(x)) \quad (2b)$$

where h is the step size of the integration, then equation set 3.1) is solved by successive applications of the formulas:

$$f_{in,\frac{1}{2}}(x) = f_{in,0}(x) + \tfrac{1}{2} h f'_{in,0}(x) + h^2/24 (4 F_{i,0} - F_{i,-\frac{1}{2}})$$

$$f_{in,1}(x) = f_{in,0}(x) + h f'_{in,0}(x) + h^2/6 (F_{i,0} + 2 F_{i,\frac{1}{2}})$$

$$f'_{in,1}(x) = f'_{in,0}(x) + 1/6 h (F_{i,0} + 4 F_{i,\frac{1}{2}} + F_{i,1}).$$

Comparison of equation 3.1) to equation 2.21a), the homogeneous form of equation 2.19), shows that the function $F_{i,j}$ is merely the sum of coupling terms:

$$2\mu_{12}/\hbar^2 \sum_{k=1}^{W} V_{ik}(x) f^h_{kn}(x)$$

formed from the eigenfunction series representation of the solution to the partial differential equation and evaluated at the j^{th} integration point, $x = x_0 + jh$.

The definition of $f'_{in,j}(x)$ is that of the standard derivative,

$$f'_{in,j}(x) = \partial/\partial x (f_{in}(x))_{x=x_0+jh}$$

The point x_0 should not be confused with the point x° of section 2. The notation x_0 is used here to denote an arbitary point along the x axis at which the integration was initiated.

While de Vogelaere's method is a Cauchy technique, the applications of this method to rotational scattering have not included any renomalization formalisms (Le68b). This particular propagation sequence has sufficient stability to solve some problems without developing linear dependence in the solution set.

A second method which makes specific use of the absence of a first derivative term in the closed, coupled equations of the scattering problem is the reference function technique, first applied to the inelastic scattering problem by Gordon (Go69). This mechanism for integrating the coupled, differential equations makes use of a reference equation to develop sectionally valid solutions to the full equation set.

The reference equation for the inelastic scattering equation is a second order differential equation with a polynomial approximation for the potential term. The two basic approximations for the potential term are to represent $V_{pj}(x)$ as a constant or a linear function of x,

$$V_{pj}(x) = c_{pj} \tag{3a}$$

or

$$V_{pj}(x) = d_{pj}x + e_{pj}, \tag{3b}$$

over a small region of the x axis. The total homogeneous

equation then reads

$$\left\{ {}^{\partial^2 f_{pn}(x)}/_{\partial x^2} - {}^{2\mu_{12}}/_{\hbar^2} \sum_{j=1}^{W} c_{pj} f_{jn}(x) \right\} = 0 \qquad (4a)$$

or

$$\left\{ {}^{\partial^2 f_{pn}(x)}/_{\partial x^2} - {}^{2\mu_{12}}/_{\hbar^2} \sum_{j=1}^{W} \left[d_{pj} x + e_{pj} \right] f_{jn}(x) \right\} = 0. \qquad (4b)$$

The two relationships 3.4a) and 3.4b) possess analytic solutions. These solutions are the harmonic functions and the Airy functions,

$$\{ \sin(kx), \cos(kx) \} \qquad (5a)$$

and

$$\{ \mathrm{Ai}(kx), \mathrm{Bi}(kx) \}, \qquad (5b)$$

respectively. These reference functions are used to approximate the true solution to equation 2.19) in a small segment of x,

$$a \leq x \leq b,$$

chosen such that the polynomial expansion of the potential matrix element given in equation 3.3) holds to within a fixed error, ϵ.

When all parts of the x axis contained in the interaction zone have been used to create a reference function solution to equation 3.4), these separate solution parts are meshed into one continuous solution.

Since Gordon first applied the reference function technique to the rotationally inelastic scattering of three atoms in 1968, this method has gained rapid acceptance as a mechanism for solving the coupled scattering equations. In 1970, Krauss and Mies (Kr70) published a calculation of electron-diatom cross

sections about the 2 e. v. resonance of $e^{-}N_2$ which were prepared with reference function methods. The method has been applied to rotational, three atom scattering by Wolken, Miller and Karplus (Wo72), to rotational, vibrational, three atom scattering by Wagner (Wa72), and to reactive, collinear, three atom scattering by Middleton and Wyatt (Mi72). This integration technique has also appeared (Al72) as part of a formalism for solving time dependent Hartree-Fock perturbation equations.

Inhomogeneous Equations of the Method of Subtracted Asymptotics

The inhomogeneous equations of the Method of Subtracted Asymptotics have not been specifically treated in the previous discussion of the numerical methods. For the de Vogelaere method of solving the coupled differential equations, the inhomogeneity causes no change in the formalism. The inhomogeneous function is absorbed into the functions F_i of equation 3.1) and a particular solution to the non-homogeneous equation is generated.

Gordon's reference function formalism is also capable of solving the non-homogeneous problem but additional theory is needed to obtain a particular solution to equation 2.19). The methodology which enabled the Gordon technique to solve an inhomogeneous problem is termed the Variation of Constants technique (Co61a).

Before a Variation of Constants formula may be used for an inhomogeneous, ordinary differential equation, the independent

solutions to the homogeneous form of the equation must be known. The reference functions of equation 3.5) provide a homogeneous solution set which meets this requirement.

Using the homogeneous solution sets, the general solution to the coupled equations is posed as

$$u_{pn}(x)\,\sin(k_p x) + v_{pn}(x)\,\cos(k_p x) \qquad (6a)$$

or

$$u_{pn}(x)\,\mathrm{Ai}(k_p x) + v_{pn}(x)\,\mathrm{Bi}(k_p x), \qquad (6b)$$
$$p = 1 \text{ to } W.$$

The insertion of the functions of equation 3.6) into the appropriate relationship of equation 3.5) yields a first order, coupled equation for the variable multipliers $u_{pn}(x)$ and $v_{pn}(x)$. Once these equations are integrated, a particular solution to the inhomogeneous problem is known.

If a Cauchy method is used to solve the coupled equations, then a particular form of the analysis equations must be used to define the unknowns of the scattering problem. All of the analysis equations of section 2 should be posed as relationships between the value or derivative of the interaction zone solution, $\Phi_n + \chi_n$, and the respective value or derivative of the asymptotic solution, Ψ_n. These equations are imposed at the two lines which mark the start of the asymptotic region, x° and $x^{\circ\prime}$.

Dirichlet Methods

The most common Dirichlet technique for a homogeneous, ordinary differential or elliptic, partial differential equation is the

finite difference method (Ca59b). The solution to the differential equation set is obtained by approximating the result of all differential operators by a linear combination of the solution to the equation set. Thus, for example, a second order differential operator at the point x_j becomes (Ab68),

$$h^2 \, \partial^2 f(x_j) / \partial x^2 = f(x_j - h) - 2 f(x_j) + f(x_j + h) \qquad (7)$$

where h is the step size of the integration.

This process of replacement of differential operators by linear combinations of the solution is continued at all points of the variable within the boundaries of the region treated. At the boundaries, the solution components $f(x_b)$ are known by boundary conditions and thus, the operator expressions can be solved recursively for a total solution.

Finite difference techniques were used by Mazur and Rubin to solve the time dependent Schrödinger equation for a collinear, reactive collision in 1959. Mortensen and Pitzer (Mo62, Mo68) also treated the reactive, collinear collision with finite difference techniques. Diestler, Gutschick and McKoy (Di69a, Di68b, Gu70) treated both the inelastic and the reactive quantum equations for three atom collisions with a discritization technique. However, this numerical method is very expensive, very slow and superceded by another far better formalism for solving the inelastic scattering equations. Hence, it was not considered as a means of solving equation 2.19).

A method far more effective than the finite difference ap-

proach to the Dirichlet problem was developed by B. Numerov in 1933 (Nu33). As is true of the Gordon and de Vogelaere methods, this integration formula is specificly adapted to sets of coupled differential equations which lack a first derivative.

The Numerov method was developed to treat the orbits of comets and planets (Col0, Ja24) but the occurence of second order differential equations throughout physics lead to an application of this technique to arbitary sets of coupled equations (Ha57, Ha65). If the notation

$$\Upsilon_{ik} = {}^{2\mu_{12}}/_{\hbar^2} V_{ik}(x) \tag{8a}$$

is introduced for the elements of the potential matrix, then the Numerov propagation equation for equation 2.19) can be written

$$\sum_{k=1}^{W} (\delta_k^i - {}^{h^2}/_{12}\,\Upsilon_{ik}(x_{m+1}))f_{kn}(x_{m+1}) = \sum_{k=1}^{W} (2\delta_k^i + {}^{5}/_{6}\,h^2\Upsilon_{ik}(x_m))f_{kn}(x_m) + \sum_{k=1}^{W} (-\delta_k^i + {}^{h^2}/_{12}\,\Upsilon_{ik}(x_{m-1}))f_{kn}(x_{m-1}) \tag{8b}$$

where h is the step size of the integration, and

$$x_{m+1} = x_0 + (m+1)h. \tag{8c}$$

Equation 3.8) is one portion of a matrix relation that determines W independent solutions, $\{\{f_{jn}(x),\ j=1 \text{ to } W\};\ n = 1 \text{ to } W\}$, in one integration.

The Numerov method has been applied to several branches of scattering theory. The method was applied to quantum physics in the late 1950's by three separate groups seeking to solve the radial Schrödinger equation (Ru56, Sk59, Co61b). Two studies

by Marriott have been particularly important in initiating the scattering application of this technique. In 1957, Marriott published (Ma57) a study of the decay of electronically excited helium under electron bombardment in which the integro-differential scattering equations were solved by the backward substitution method. Later Marriott (Ma64) applied this same technique to the problem of collisional excitation of carbon monoxide. A slight adjustment of this formalism yields the Numerov method and, in 1965, Barnes, Lane and Lin (Ba65) reported electron excitation cross sections for sodium prepared using this technique.

The more general formalism for solving the equations representing the perturbation of systems with $2p^q$ and $3p^q$ configurations by an electron, with the Numerov technique was published by Smith, Henery and Burke (Sm66) in 1966. The work of Smith, Henery and Burke was the final stepping stone which lead to the application of the Numerov method to diatomic collision problems. Lane and Geltman (La67) performed calculations on rotational excitations of diatomic molecules by electrons with the Numerov method and Allison and Delgarno (Al67) used this technique to solve atom-diatom rotational excitation equations.

Inhomogeneous Equations

An inhomogeneous function in the set of coupled differential equations treated merely adds one known term to the right hand

side of equation 3.8b) for the Numerov technique. Thus, this method can also be used to solve the inhomogeneous differential equations.

Another Dirichlet method for solving the inhomogeneous equations of the Method of Subtracted Asymptotics that was given serious consideration was the use of orthoginal functions to create the particular solution needed by expansion in a series of known functions. The functions chosen for this approach to the inhomogeneous problem were the set of Chebyshev polynomials. These functions have been extensively used to obtain representations of solutions to differential equations (Fo68).

Analysis

To obtain a complete closed set of analysis equations from a Dirichlet solution using the analysis technique proposed by Zakhariev, equation 2.32) must be augmented by the unitarity condition given in equation 2.33) and a set of relationships based on the symmetry type of the three atom collision. If the linear collision is symmetric about the central atom,

$$A_2 + A \rightarrow A + A_2$$

or

$$AB + A \rightarrow A + BA,$$

then the R matrix symmetry condition

$$R_{ij} = R_{ji}$$

and

$$\overline{R}_{ij} = \overline{R}_{ji},$$

can be imposed to force the number of unknowns from the analysis relations to equal the number of restrictions bounding them.

If the collision is not symmetric,

$$A + BC \rightarrow AB + C,$$

then Zakhariev proposed (Ef68b) that the τ operator matrix relation

$$T_{\beta\alpha} = \int \Phi_\beta V_\beta \Psi \, d\tau,$$

be used to obtain the additional restrictions needed to calculate the reaction probabilities. The τ operator is defined in Mo65c and Wu62. Formulation of a reactive scattering problem with the aid of the τ operator allowed Baer and Kouri (Ba71, Ba72a) to obtain reaction probabilities for a very simple, predominately analytic, model problem. In general, however, the use of the τ operator or its matrix equivalent is not a practical numerical technique.

The expansion analysis represented by equations 2.35) and 2.37) can be applied to a Dirichlet scattering solution by satisfying the decomposition expression, equation 2.35), at two points. This specifies the constants in the expansion of each part of the total interaction solution, allowing equation 2.37) to be solved for the $\underset{\sim}{R}$ matrix elements.

Conclusions

Only three numerical integration schemes are sufficiently efficient to be used to solve the coupled equations developed in the execution of the Method of Subtracted Asymptotics. These

schemes are the de Vogelaere method, the Gordon method and the Numerov method.

The Gordon method and the Numerov method were given serious consideration as possible formalisms for solving equation 2.19). Because of its sectional analytic solutions and, therefore, because of the ability to use the variation of constants technique as a solution to the inhomogeneous equations considered, the Gordon method was chosen as the numerical integration technique used for this study of the Method of Subtracted Asymptotics.

4: Applications of the Method of Subtracted Asymptotics

The Method of Subtracted Asymptotics was originally investigated to determine if it could be effectively applied to the problems of electronically adiabatic, three atom, reactive collisions. There are several light atom reactions which apparently contain significant quantum effects. Studies by Miller and Rankin (Mi71a) have compared classical H-Cl_2 results to the quantum studies of Miller and Light (Mi71b), using the same potential surface, and have found that the classical and quantum results disagreed. Similar work has been done on the reaction F + H_2 (Sc73) and the exchange reaction H_2 + H (Bo71, Bo73).

Three reactions have thus indicated that quantum phenomena control some of the reactions currently being investigated by molecular beam techniques(An69, Sc70, We67). Further, a potential surface has been prepared for an H_3 reactive collision by Shavitt, Stevens, Minn and Karplus (Sh68a, Sh68b) and a potential surface has been derived for the H_2-F reaction by Bender, Pearson, O'Neil and Schaefer (Be71 , Be72).

Therefore, rapid numerical techniques which solve the reactive, three atom Schrödinger equation will allow an extensive investigation of the exact processes involved in a chemical reaction. The Method of Subtracted Asymptotics, an untested method in chemical scattering, seemed to have a possibility for solving the equations for a collinear, reactive collision in a minimum amount of time. This prospect of a rapid numerical method initiated this

investigation.

While later investigations were to be aimed at the reactive systems previously mentioned, the initial calculations attempted with M. S. A. were done on a very simple model problem. The model system selected was the one dimensional collision of a particle with a two particle square well oscillator. This model system had been extensively investigated by Tang, Kleinman and Karplus (K169 , Ta69) in 1969 and Locker and Wilson (Lo70) in 1970.

The coordinates and potential surface for this system are displayed in Figure 4. A constant value was used as the interaction potential for the three colliding atoms and the interaction region eigenfunction expansion set, $\{\Lambda_k(x_{ij})\}$, was a set of variable width square well functions. The formulas for the eigenfunctions in the x_{23} direction, as a function of x', are

	x' value	x_{23} maxima
1)	$0 \le x' \le x_0/h_2$	$x_{23} = -(h_6/h_8)x'$
2)	$x_0/h_2 < x' \le x'_0$	$x_{23} = (x_0 - h_2x')/h_4$
3)	$x'_0 < x'$	$x_{23} = \ell'$

	oscillator function
1)	$(-2h_8/h_6x')^{\frac{1}{2}} \sin(-m\pi h_8/h_6x'x_{23})$
2)	$(2h_4/(x_0 - h_2x'))^{\frac{1}{2}} \sin(m\pi h_4/(x_0 - h_2x')x_{23})$
3)	$(2/\ell')^{\frac{1}{2}} \sin(m\pi/\ell' \; x_{23})$

where ℓ' is the width of the oscillator's well, x° and $x^{\circ\prime}$ are defined in Figure 4 and the h_i mass constants are

$$M = m_1 + m_2 + m_3$$

$$h_1 = -m_1/(m_1 + m_2)$$

$$h_2 = -m_3/(m_2 + m_3)$$

$$h_3 = -[m_1 m_2 M/m_3]^{\frac{1}{2}}/(m_1 + m_2)$$

$$h_4 = \{(m_1 + m_2)[m_3/m_1 m_2 M]^{\frac{1}{2}} - m_3/(m_2 + m_3)[m_1 m_3/m_2 M]^{\frac{1}{2}}\}$$

$$h_5 = (m_1 + m_2)^{-1}(m_1 m_2 M/M_3)^{\frac{1}{2}}$$

$$h_6 = -(m_2 + m_3)^{-1}(m_2 m_3 M/m_1)^{\frac{1}{2}}$$

$$h_7 = -m_1/(m_1 + m_2)$$

$$h_8 = -m_3/(m_2 + m_3)$$

A Gordon propagator using a constant potential term (see equation 3.3a) was programed for this system. The programing and numerical treatment of this model were probed and adjusted for a considerable period but no convergence pattern or valid results could be obtained from the integration program. Because the integrator for this problem was a very extensive and involved package, no direct cause could be established for the failures of the computer program.

Since the Tang, Kleinman and Karplus square well reaction probabilities could not be duplicated by integration of the equations of the Method of Subtracted Asymptotics, it was concluded that an error or a numerical problem existed at some point in the formulation of the scattering equations. However, the complexity of the Tang, Kleinman and Karplus (T.K.K.) model obfuscated the difficulty in the numerical solution of the collision equations. Hence, a simpler model problem was selected for treatment by M.S.A. It was hoped that the necessary clarifying

insights needed to correct the treatment of the T.K.K. model could be obtained from a simpler system. This hope was ill-founded and as the latter portion of this section will show, M.S.A. or eigenfunction expansion cannot practicably be applied to the scattering problem.

The second model chosen for consideration was the infinite central mass form of the particle, two-particle-square-well collision. This model was first used by Hulbert and Hirschfelder (Hu43) to depict a chemical reaction independent of rotational and electronic excitations. It has since been investigated by several researchers using different techniques (Ro70 , Ba72 , Di69).

Upon taking a limit on a three particle system as the central mass goes to infinity, a great deal of simplification occurs in the equations governing the collision. The hamiltonian for this collision, when posed with a constant interaction potential V_o, is

$$\mathcal{H} = \left[{}^{\partial^2}/_{\partial x^2} + {}^{\partial^2}/_{\partial y^2} - {}^{2}/_{\hbar^2}(V_0) \right]. \qquad (1)$$

The scaled coordinate set for this system is defined by Figure 5. With the channel widths taken as π for both entrance and exit channels, the eigenfunction equations for the asymptotic wave-functions describing the two possible diatoms are

$$\left[{}^{\partial^2}/_{\partial x^2} - \epsilon_j \right] \overline{\phi}_j(x) = 0 \quad \overline{\phi}_j(x) = ({}^{2}/_{\pi})^{\frac{1}{2}} \sin(jx), \qquad (2a)$$

$$\left[{}^{\partial^2}/_{\partial y^2} - \epsilon_j \right] \phi_j(y) = 0 \quad \phi_j(y) = ({}^{2}/_{\pi})^{\frac{1}{2}} \sin(jy), \qquad (2b)$$

$$\epsilon_j = {}^{j^2}/_{2}. \qquad (2c)$$

Because of the geometry apparent in Figure 5, the set of interaction region eigenfunctions, $\{\Lambda_j(y)\}$, coincides with the asymptotic entrance channel eigenfunctions, $\{\phi_j(y)\}$. The regularity of this geometry and the use of a constant interaction potential also removes the subchannel coupling terms which make the independent solutions of equation 2.19) full vectors. The independent solutions for the infinite central mass model are single functions and the full set of solutions forms a diagonal matrix.

The boundary condition function, $\Phi(x, y)$, also reduces greatly for this model. Let the total reduced energy for the collision be taken as

$$0.5 \leq E \leq 2.0 \qquad (3)$$

where

$$E = \left(8M'\pi^2/h^2\right) E'.$$

Here M' is the mass of the free particle, taken as 1 for these calculations, and E' is the absolute energy. Under this energy limit, only one subchannel is open in each channel. This implies that the sum over all subchannels in equation 2.12) consists of only one term so that $\Phi(x, y)$ becomes

$$\Phi_1(x, y) = \overline{R}_{1n} \sum_{i=1}^{M} y D_{11}^{i} \overline{\phi}_1(x) g_i(y) \qquad (4)$$

For the work with the infinite, central mass model, the functions $g_i(y)$ were taken to be powers of the variable y when the Zakhariev analysis technique was used. Thus

$$g_i(y) = y^{i-1}$$

and

$$\Phi_1(x,y) = \overline{R}_{1n} \sum_{i=1}^{M} D_{i1}^{i} \overline{\phi}_1(x)\, y^{i}. \qquad (5)$$

Operating on $\Phi_1(x,y)$ with $(\mathcal{H}-E)$ shows that the inhomogeneity generated by this function is a simple polynomial-oscillator function product. This inhomogeneity is to be removed by a solution created through an expansion in the eigenfunctions of the interaction region. Assuming Zakhariev's direct matching analysis formulas will be used to determine the elements of the R matrix, the restrictions which must be met to create a balanced, well posed set of equations for solving the scattering problem will be investigated at this point. Concentrating on how the analysis formalism effects the X portion of the Method of Subtracted Asymptotics solution will show that the term by term Zakhariev analysis cannot solve the scattering problem.

Equation 2.32) shows the matrix form of the term by term analysis. In order to expose the full significance of this analysis formalism, the energy restriction of equation 4.3) will momentarily be dropped. There will be P open entrance subchannels, Q open reacted subchannels and W subchannel terms used in the X expansion in the equations formulated here.

Consider the entrance channel relation, equation 2.32a) and the derivative with respect to x of this relation. If one distinct element of the set of (W+w) entrance channel asymptotic eigenfunctions is multiplied into these two equations and the result is

integrated over all y, two sets of subchannel equations are obtained. The set from equation 2.32a) contains $W \times P$ separate restrictions while the equation set obtained from the derivative of equation 2.32a) will contain $(W+w) \times P$ restrictions on the unknowns of the scattering problem.

This process of projecting the matrix analysis equations on the asymptotic eigenfunctions of the reaction must be repeated at the boundary line of the reacted channel. There $(Q+q)$ subchannel eigenfunctions will be used to convert equation 2.32b), and its derivative with respect to y, into two sets of equations. Equation 2.32b) provides $Q \times Q$ equations while its derivative breaks down into $(Q+q) \times Q$ equations.

If the unitarity condition of equation 2.33) is imposed, it provides P additional equations.

The unknowns of this problem are the $W \times P$ elements of the recombination matrix, $\underset{\sim}{C}$; the $P \times P$ elements of the $\underset{\sim}{R}$ matrix; the $Q \times P$ elements of the $\underset{\sim}{\bar{R}}$ matrix and the $M \times Q \times Q$ elements of the $\underset{\sim}{D}$ matrices contained in Φ.

To obtain a solution that is not a least squares fit to the set of equations created in this analysis, the number of equations must equal the number of unknowns in the equations. This implies that

$$(q-P) \times Q + (W+1+w-P) \times P = (M-2) \times Q^2. \qquad (6)$$

Equation 4.6) displays the crux of the problem in Zakhariev's analysis. If the number of eigenfunctions used to create the X

solution is to be increased, then beyond the point at which equation 4.6) forces q and w to be set to zero, increases in W mean increases in M, the number of terms in $\Phi_1(x, y)$. Since $\Phi_1(x, y)$ does not satisfy the differential equation, the additional terms in this function appear in the inhomogeneity contained in the equation for χ.

Thus, $\chi(x, y)$ is required to solve a more extensive inhomogeneous equation. Obviously, the greater complexity of the χ equation will necessitate the use of more eigenfunctions in χ to achieve a given accuracy. This makes any effort to obtain a converged χ function cyclic. To calculate a more accurate χ, the expansion level, W must be increased. Because of equation 4.6), this correspondingly increases M, making $\Phi_1(x, y)$ more complicated and thereby lowering the accuracy of $\chi(x, y)$.

If this cyclic process is to be avoided, a limit must be set on M. Such an expansion maxima totally destroys any possibility of achieving an accurate solution to the scattering equation because sufficient eigenfunctions cannot be introduced into χ. Table 1 lists a series of results that were obtained with the Zakhariev form of the M. S. A. equations. The results show the rapid divergence of this type of analysis. The small number of eigenfunctions used in this calculation do not allow the probabilities to approach the known values for the infinite central mass, square well, three particle collision.

The Expansion Analysis

The expansion analysis characterized by equations 2.35) and 2.37) was developed to circumvent the major flaw of the term by term analysis; namely, the strict restriction of the degree of expansion in X by other portions of the scattering solution. An analysis technique which would allow an arbitary number of eigenfunction terms to be placed in X was created by the asymptotic decomposition of all functions contributing to X at the entrance boundary.

Again using the P, Q, W notation for the number of subchannels appearing in the Method of Subtracted Asymptotics solution, the "balanced" equation set condition for the expansion analysis becomes:

$$q\,P = P^2 + 2\,Q^2 - P\,Q. \qquad (7)$$

The degree of expansion of the X function, W, does not appear in this equation. It is unlimited and can adopt any value needed to create a converged form of the entrance channel solution. The integer M also does not appear in equation 4.7). It is therefore independent of any efforts made to analyse the scattering solution and can be given any convenient value which allows a continuation of Φ across Γ, the eigenfunction boundary. A value of two was chosen for M.

The $\Phi_1(x,y)$ function used with the expansion analysis was:

$$\Phi_1 = y\left[\, D_{11}^1 \sin(K_1^r\, y) + D_{11}^2 \cos(K_1^r\, y)\right] \overline{\phi}_1(x)\, \overline{R}_{11} \qquad (8)$$

The set of homogeneous functions which satisfy equation 2.21a)

as altered for the infinite central mass model are the harmonic and hyperbolic functions defined in (Di70). The open and virtual particular solutions to the inhomogeneous equation resulting from the Φ function of equation 4. 8), are shown in Table 2.

These functions were created by Cauchy propagation and were analysed under the expansion analysis formulas of equation 2. 35). The manipulation of these solutions dictated by the expansion analysis formulas was carried out with several numerical techniques. The techniques were changed when each method failed to provide the needed convergence capacity required to solve the analysis equations.

The first formula programed to solve the nonlinear analysis equations was Newton's method (Bo66). The iterative formulation of Newton's equations with a Jacobian adjustment of the initial solution guesses failed to converge when more than two eigenfunctions were used in the χ expansion.

With the failure of the Newton technique, an algorithm developed by M. J. D. Rowell (Ra69a) was used to solve the analysis problem. This algorithm used several gradiant methods to create a numerical approximation to the solutions of the equations it treated. The additional numerical capacity of this subroutine did allow larger expansion forms of the χ solution to be solved. However, even a six subchannel calculation containing one open subchannel in each rearrangement channel and five virtual substates in the χ expansion, yielded probabilities which

bore no relation to the published values (Ta69, Di69).

A final technique that was used to check the results of the iterative methods already discussed was basic factorization and reduction of the analysis equations. This was accomplished by symbolic manipulation of the analysis relations using the computer language Reduce (He70). The resulting factored equation was solved with Muller's root sorting method (Mu56).

After all of the analysis investigations had failed to yield the expected answer for a low energy, one open subchannel per channel, infinite central mass collision, the route of this investigation was altered so that the problem could be approached with a goal of determining the possibility of convergence of this method to the published result. Since the Method of Subtracted Asymptotics creates an eigenfunction expansion solution to the Schrödinger equation, the degree of the expansion needed to solve the partial differential equation to a given accuracy was calculated.

If the total solution to the Schrödinger equation is $\Phi + X$, then the error integral

$$\epsilon^2 = \int [(\mathcal{H} - E)\Phi + (\mathcal{H} - E)X]^2 d\tau \qquad (9)$$

represents the error over the entire interaction region for the solution to the Schrödinger equation. Equation 4. 9) is a function relationship and is independent of any constants that must be determined through solution analysis. Hence, the accuracy of the solution prepared by the Method of Subtracted Asymptotics

can be tested at various levels of expansion for the χ function.

Other calculations on the three atom scattering problem have established the accuracy bounds on numerical scattering solutions that must be met to provide valid results for the scattering parameters. By applying these accuracy criteria to the error values determined through equation 4.9), the degree of expansion needed to obtain a viable solution to equation 2.19) can be established.

The calculations of Wagner (Wa72) and Truhlar (Tr70a) have been conducted with solutions of less than 4% error. As an upper bound on the accuracy that must be demanded of the total solution, a value of 5% relative error in the numerical solution was chosen. The formula used to calculate the relative error contained in the Method of Subtracted Asymptotics solution was

$$\epsilon_r = \left\{ \int \left[(\mathcal{H}-E)\Phi + (\mathcal{H}-E)\chi \right]^2 d\tau \right\}^{\frac{1}{2}} / \int (\mathcal{H}-E)\Phi \, d\tau .$$

An energy spectrum for the relative error for three distinct levels of expansion of the χ function is shown in Figures 6, 7, and 8. The constant potential was set to zero for these calculations. After the inclusion of 5 subchannels in the expansion, Figure 6 shows that the total solution has, at a few points of the energy spectrum, achieved the accuracy needed to solve the scattering problem. Figures 7 and 8 show that the basic 5% relative error criteria is not met at all points of the energy spectrum until 12 eigenfunctions are included in the expansion.

Thus, to prepare an energy spectum for the infinite central mass, square well collision at energy values such that one subchannel is open in each channel, requires an eigenfunction expansion which includes between 7 to 11 virtual states, depending on the energy of the calculation.

The analysis of such a large set of solutions, even for a one open subchannel case, is not possible. Numerical stability problems in the treatment of the analysis equations become very pronounced when large numbers of expansion eigenfunctions enter the equations. It becomes completely impossible to determine the primary unknowns, the R matrix elements, in these equations because the elements R_{ij} or $\overline{R}_{ij}$ are of order unity in an equation set dominated by large virtual wavefunctions.

Finally, a numerical method which must introduce approximately nine virtual states for each open state that appears in a scattering calculation is totally useless as a practical solution mechanism. Such an eigenfunction spectrum can be completed (Wi65, Co61b, Me70) but other methods mentioned heretofore for treating the reactive scattering problem can solve the collision equations with much less effort. On the basis of these stability and efficiency problems, the effort to solve the scattering equations with the Method of Subtracted Asymptotics was abandoned.

The major flaw in the method proposed by Efimenko, Zhigunov and Zakhariev and herein shown to be an eigenfunction

expansion technique, is that the introduction of an inhomogeneity into the Schrödinger equation by the boundary condition solution, Φ, mandates that a large number of states must be included in the expansion solution, χ. The degree of eigenfunction expansion needed to satisfy the total equation is so large that gross efficiency and propagation problems can not be avoided. This feature of the method is discussed in detail in the next section.

5: Conclusions

The major motivation for this research into the Method of Subtracted Asymptotics was to obtain a treatment of the reactive scattering problem which could use asymptotic eigenfunctions to reduce the quantum partial differential equation to a series of coupled equations. These coupled equations could then be rapidly solved by a propagator technique.

The Method of Subtracted Asymptotics has been abandoned because it cannot meet these criteria. The method fails in each of the particular aspects for which it was investigated.

The Method of Subtracted Asymptotics will not permit the solution of the Schrödinger equation with asymptotic channel eigenfunctions within the interaction zone of the three particle collision. Because this technique is an application of the formalism of eigenfunction expansion, the eigenfunctions which are used to solve the wave equation must be calculated at each point of the channel being treated. The need to generate an eigenfunction set $\{\Lambda_j(x)\}$ for each step taken down the propagation channel makes this method far more involved and cumbersome than it was originally expected to be.

Perhaps the most serious difficulty with this method arises from the need to solve an inhomogeneous equation using an eigenfunction expansion method. Until the full solution to the wave equation is made homogeneous, the function $\Phi+\chi$ cannot possibly solve the Schrödinger equation. Thus, until the expansion, χ,

becomes extensive enough to virtually completely remove the function $(\mathcal{H}-E)\Phi$ from the differential equation, the Method of Subtracted Asymptotics solution will remain invalid. Since the inhomogenaity contains both the Laplacian of Φ and the product of a normally very convoluted potential surface and Φ, the expansion for X will always be of high degree.

To solve such an extended eigenfunction expansion for the scattering problem would require a numerical propagation technique of exceptional stability. While transform techniques allow a large expansion problem to be solved, the efficiency of such propagation is still quite low and therefore, the Method of Subtracted Asymptotics will, a priori be significantly slower than existing techniques (Mi72, Ra69b, Mi71a, Mi71b, Sc73).

When the numerical solution to the coupled equations created by this method are complete, the final difficulty of analysis must be faced. The general formalism of eigenfunction expansion is usually used when just a solution is sought to a partial differential equation. Thus, a function satisfying the partial differential equation is the sole goal of most applications of eigenfunction expansion. In the scattering problem, a solution to the differential relationship is needed but the constant elements of the R matrix are the ultimate goal of a scattering calculation. Major problems arise when an attempt is made to remove the small constants of the R matrix from the total two part solution. This solution is dominated by the large virtual eigenfunction terms of the X expansion and these

terms obscure the desired results.

While the Method of Subtracted Asymptotics can be dismissed as a practical method, the formalism of this method, with the eigenfunction adjustments discussed in section 1 added, can be used to treat certain phenomena in rearrangement scattering if appropriate caution is exercised. Caution is called for in the application of this formalism because of the needs of this method in the interaction region of the reactive encounter.

In the interaction zone, this method depends on a specific set of functions, the $\{\Lambda_j(x)\}$. To apply the Method of Subtracted Asymptotics to a particular problem or a distinct class of problems, the potential surface of the interaction zone must first be carefully defined and bounded. It must then be proven that there exists a set of eigenfunctions $\{\Lambda_j(x)\}$ on this surface with some chosen boundary, Γ (see Ti62). Further, before any theoretical manipulations can be undertaken, it must be shown that the eigenfunction spectrum is complete (Ka57).

Having established existence and completeness for the eigenfunction set $\{\Lambda_j(x)\}$, it must finally be established that there exists a convergent (Br26a) eigenfunction expansion in $\{\Lambda_j(x)\}$ of any solution to the scattering equation. If at all possible and, in all probability, if anything of any value is to be proven about the scattering solution, it should also be established that the eigenfunction expansion is uniformly convergent (Br26b). Only when all of these criteria are met can a theoretical investigation of the scattering problem be undertaken.

The Method of Subtracted Asymptotics has been used by several investigators (Za71, Za70, Ki72, Au69, Ef70) to establish bounds on the scattering matrix, to create projection operators, to apply variation principles and to manipulate other theoretical constructs in rearrangement scattering. These studies have not met any of the criteria specified above and virtually all of these works have not used the interaction zone eigenfunction set. As a result, the proofs presented in the above works are invalid and must be corrected to meet the basic requirements demanded by all eigenfunction expansion methods.

The single numerical application of the Method of Subtracted Asymptotics is the study of the low energy neutron-deuteron collision published by Zakhariev, Pustovalov and Efros (Za68a). The set of expansion functions, $\{\Lambda_j(x)\}$, used in this work are the set of hyperspherical harmonics. These functions are the set of angular functions solving LaPlace's equation on a six dimensional sphere (Si66, Re69, De59, De60). They are the six dimensional anolog of the set of spherical harmonics on the standard three dimensional sphere.

The choice of hyperspherical harmonics as an expansion set corresponds to placing the expansion eigenfunction boundary, Γ, at infinity. The inhomogeneous function expansion is still bounded, however, because outside the interaction region, the inhomogeneity and the inhomogeneous solution go to zero.

A major defect in this numerical study is the use of only one eigenfunction to complete the expansion of the propagated

solution. As this work has indicated, a number of eigenfunction terms are needed to complete a solution to the equations of the Method of Subtracted Asymptotics. The decision to use only one eigenfunction term was probably not freely made by the authors but was instead, probabily mandated by analysis restrictions.

The differences found between the scattering lengths calculated in Za68a and those determined by experiment were attributed to the absence of tensor forces in the potential used in this study. While there may be some truth to this claim, inclusion of tensor nuclear forces will not remove the failures of minimal eigenfunction expansion which undoubtably play a role in the deviant results prepared for the neutron-deuteron collision.

The formalism of eigenfunction expansion, as emperically developed by Zakhariev et al, has been applied to the three particle Schrödinger equation, has been tested extensively, and has been found wanting. The Method of Subtracted Asymptotics is not a correct method, and, when corrected, is not a viable method for solving the reactive scattering equation.

Table 1

E = .55 units

Eigenfunction Terms in χ_1

W=	1		2		3		4		∞*	
	R_{11}	$\bar{R}_{11}$	R_{11}	$\bar{R}_{11}$	R_{11}	$\bar{R}_{11}$	R_{11}	$\bar{R}_{11}$	R_{11}	$\bar{R}_{11}$
M= 0									.486	.876
2	.715	.699	.715	.699	—		—			
3	—		.716	.699	.715	.699	.715	.699		
4	—		—		Diverged		.715	.699		
5	—		—		—		Diverged			

M = The number of expansion terms in Φ.

*These data from Ta69.

Open Entrance Subchannel Inhomogeneous Solution:

$$F^{I}_{nj}(x) = -{}^{w}/_{2}\left[\frac{\cos[(N - k^{e}_{j})x]}{N - k^{e}_{j}} + \frac{\cos[(N + k^{e}_{j})x]}{N + k^{e}_{j}} - \left\{ \frac{1}{N - k^{e}_{j}} + \frac{1}{N + k^{e}_{j}} \right\} \right] \sin(k^{e}_{j} x)$$

$$-{}^{w}/_{2}\left[\frac{\sin[(N - k^{e}_{j})x]}{N - k^{e}_{j}} - \frac{\sin[(N + k^{e}_{j})x]}{N + k^{e}_{j}} \right] \cos(k^{e}_{j} x)$$

Closed Entrance Subchannel Inhomogeneous Solution:

$$F^{I}_{nj}(x) = {}^{w}/_{2}\left[e^{-k^{e}_{n} x}\left\{ -k^{e}_{n} \sin(jx) - j\cos(jx) \right\}/(k^{e\,2}_{n} + j^{2}) + j/(k^{e^{2}}_{n} + j^{2}) \right] e^{k^{e}_{n} x}$$

$$+ {}^{w}/_{2}\left[e^{k^{e}_{n} x}\left\{ k^{e}_{n} \sin(jx) - j\cos(jx) \right\}/(k^{e^{2}}_{n} + j^{2}) + j/(k^{e^{2}}_{n} + j^{2}) \right] e^{-k^{e}_{n} x}$$

These functions solve the entrance channel Schrödinger equation with the reacted channel assumed function:

$$\Phi_{n}(x, y) = y\left[D^{1}_{nn} \sin(k^{r}_{n} y) + D^{2}_{nn} \cos(k^{r}_{n} y) \right] \overline{\phi}_{n}(x)$$

Definitions:

$$w = (2/\pi)^{\frac{1}{2}} M_{jn}/k^{e}_{j}$$

$$k^{e\,2}_{j} = 2/\hbar^{2}(E - V_{0}) - j^{2}$$

$$k^{r\,2}_{n} = 2/\hbar^{2}(E - V_{0}) - n^{2}$$

$$N = n\pi/\ell = n$$

$$M_{jn} = -2\,k^{r}_{n} \int \phi_{j}(y)\left[D^{1}_{nn} \sin(k^{r}_{n} y) - D^{2}_{nn} \cos(k^{r}_{n} y) \right] dy$$

Figure Captions

Figure 1: The geometry of three collinear particles with three possible coordinate sets is depicted. These coordinate pairs are $[x, x_{12}]$, $[x', x_{23}]$ and $[x_{12}, x_{23}]$.

Figure 2: A typical contour, potential energy plot of the potential surface for three arbitrary, interacting atoms with energy plotted out of the page. The coordinate set $[x_{12}, x_{23}]$ is depicted as orthogonal for convenience.

Figure 3: The three dimensional geometry of a colliding set of three particles (3b) is compared to a collinear collision, three particle geometry (3a). The notation of (3b) follows the definitions given by Miller (Mi69).

Figure 4: The geometry of the potential surface for three colliding, finite mass particles with two particles bound in an infinite square well of width ℓ is shown. The $[x, x_{12}]$ and $[x', x_{23}]$ coordinate sets are depicted as orthogonal cartesian coordinates in this figure.

Figure 5: The geometry of the potential surface for a three particle collinear collision with the bound two particle pair contained in an infinite square well is displayed. The

central particle in the collision is assumed to have an infinite mass. The scaling equations for the coordinates are $y = -(1/m_1)^{\frac{1}{2}} x_{12}$ and $x = (1/m_3)^{\frac{1}{2}} x_{23}$.

Figure 6: A plot of relative total solution error with respect to total energy of collision. Five subchannels were used in this computation. This solution has a 5% relative error for some points between E = 1.0 and E = 1.5.

Figure 7: In this relative error-energy plot, nine subchannel states have been used in the χ expansion for this calculation.

Figure 8: A total of twelve subchannel states have been included in the eigenfunction expansion to complete this plot. The solution has less than 5% total relative error at almost all points of the energy spectrum for this degree of expansion.

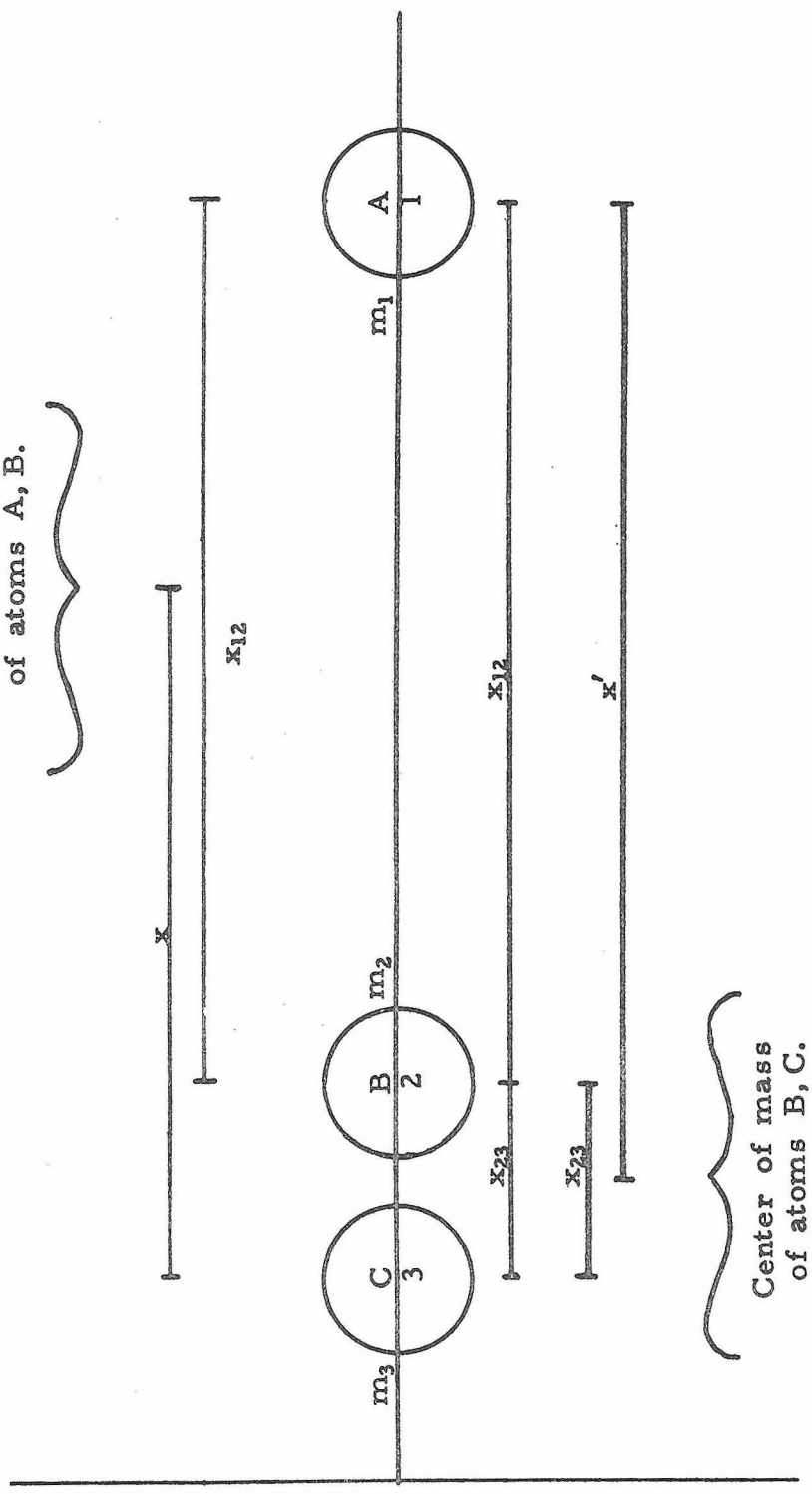

Center of mass
of atoms A, B.
x
x12
A
1
m1
B
2
m2
C
3
m3
x12
x23
x23
x'
Center of mass
of atoms B, C.

Figure 1

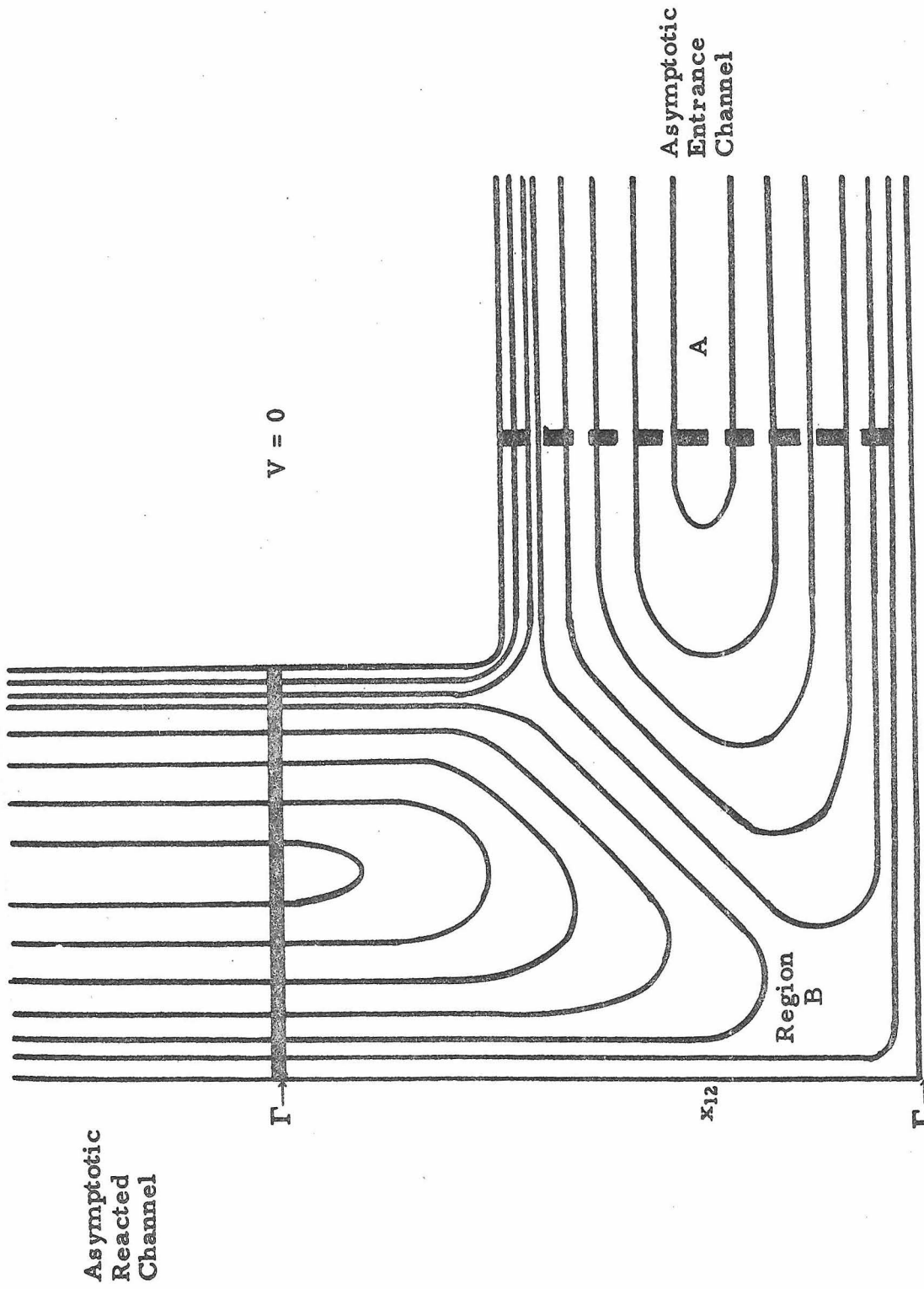

Asymptotic
Reacted
Channel
V = 0
Asymptotic
Entrance
Channel
A
Region
B
Γ
Γ
E ⊗
x_{12}
x_{23}

Figure 2

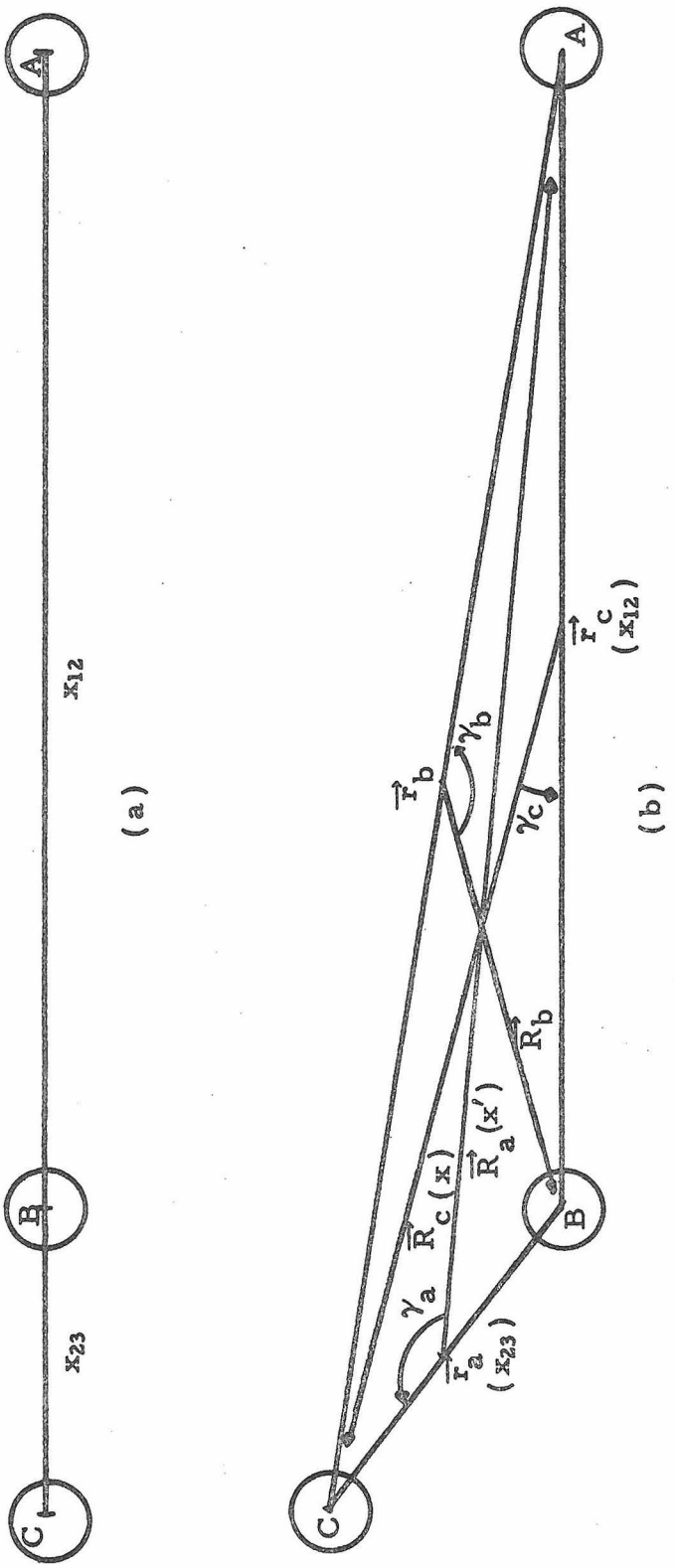

A
B
C
x_{12}
x_{23}
(a)
A
B
C
$\vec{r}_b$
γ_b
γ_c
$\vec{r}_c$ (x_{12})
$\vec{R}_b$
$\vec{R}_a(x')$
$\vec{R}_c(x)$
γ_a
$\vec{r}_a$ (x_{23})
(b)

Figure 3

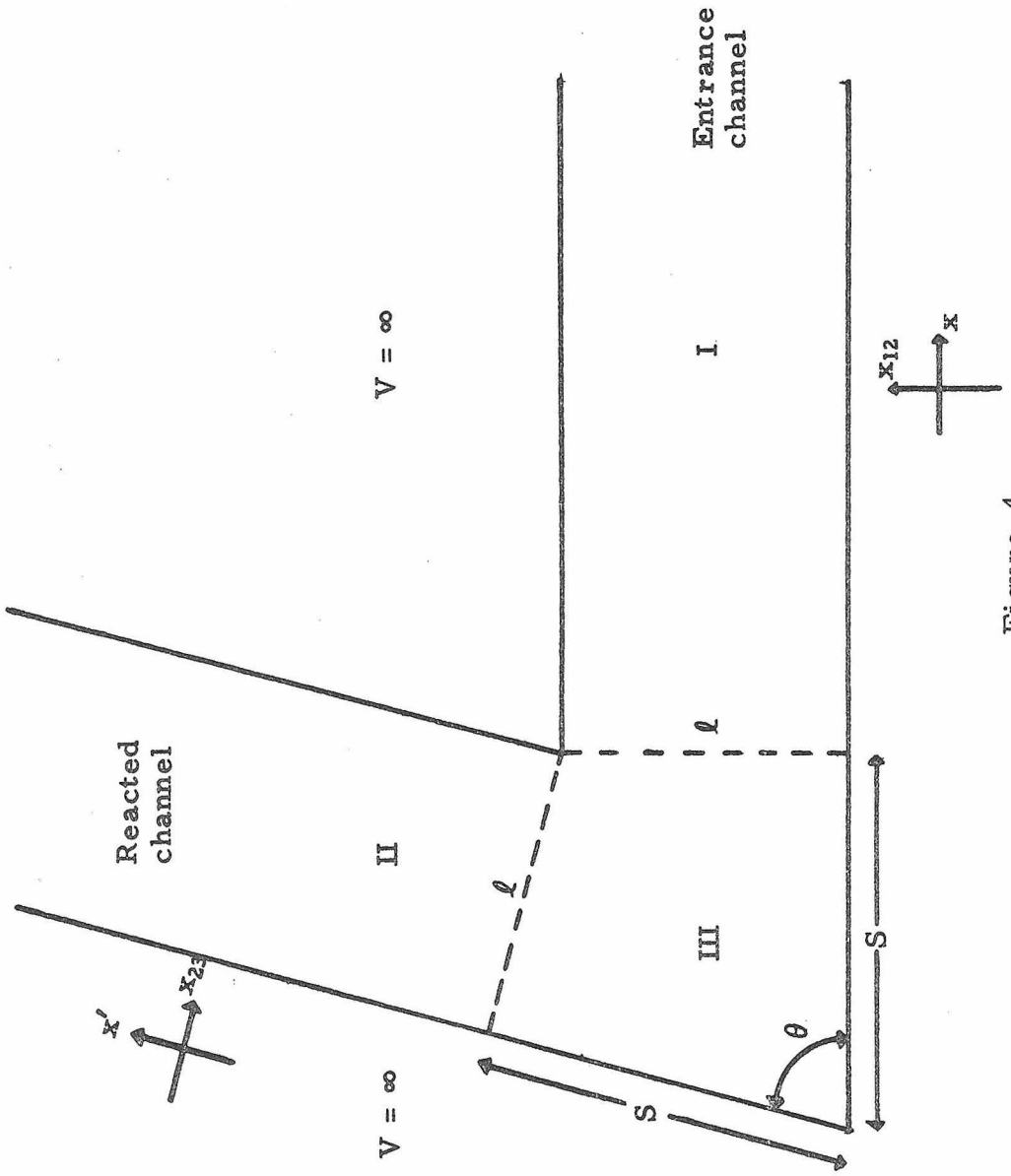

Entrance channel
Reacted channel
I
II
III
V = ∞
V = ∞
x
x12
x'
x23
l
l
S
S
θ

Figure 4

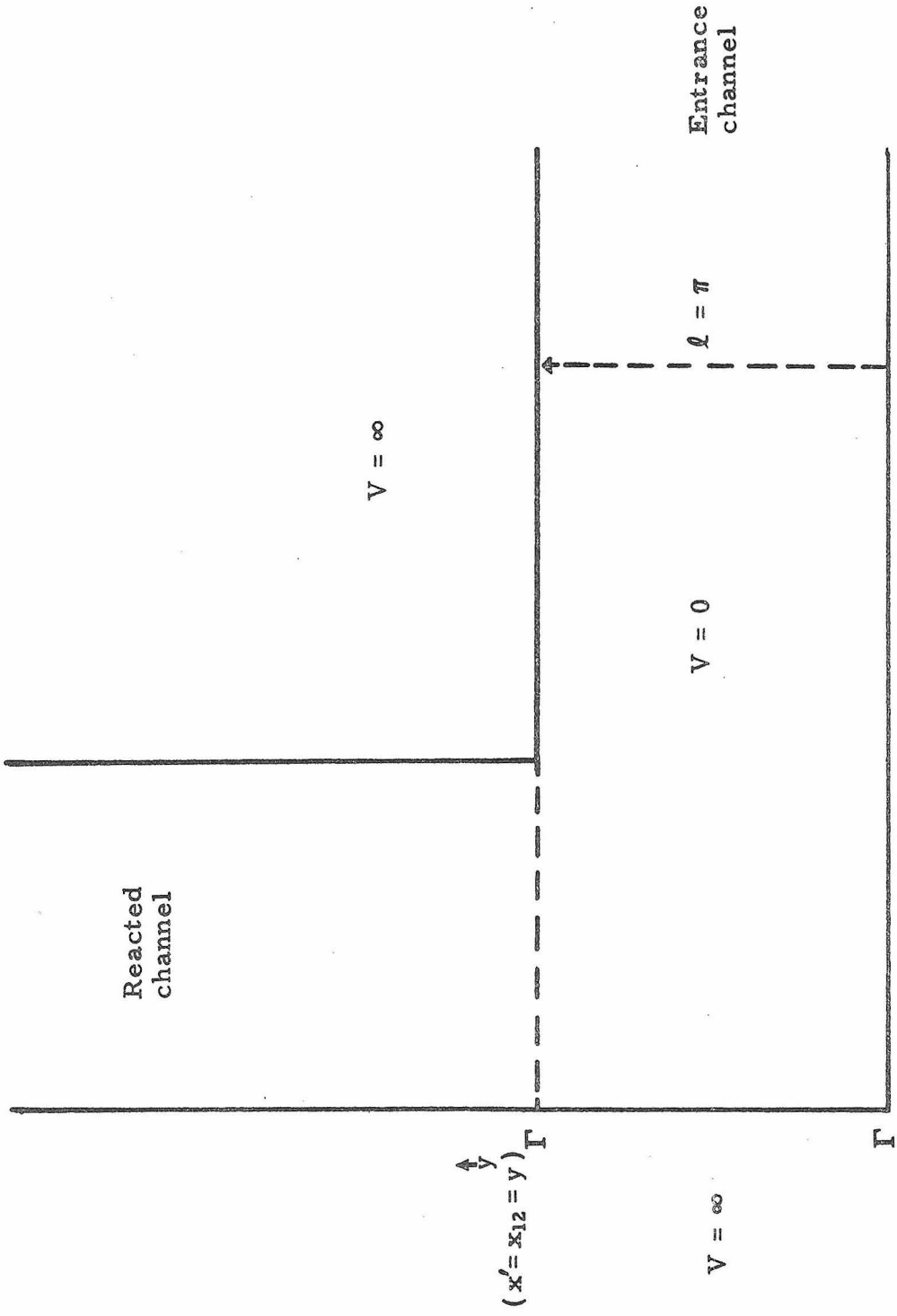


Figure 5

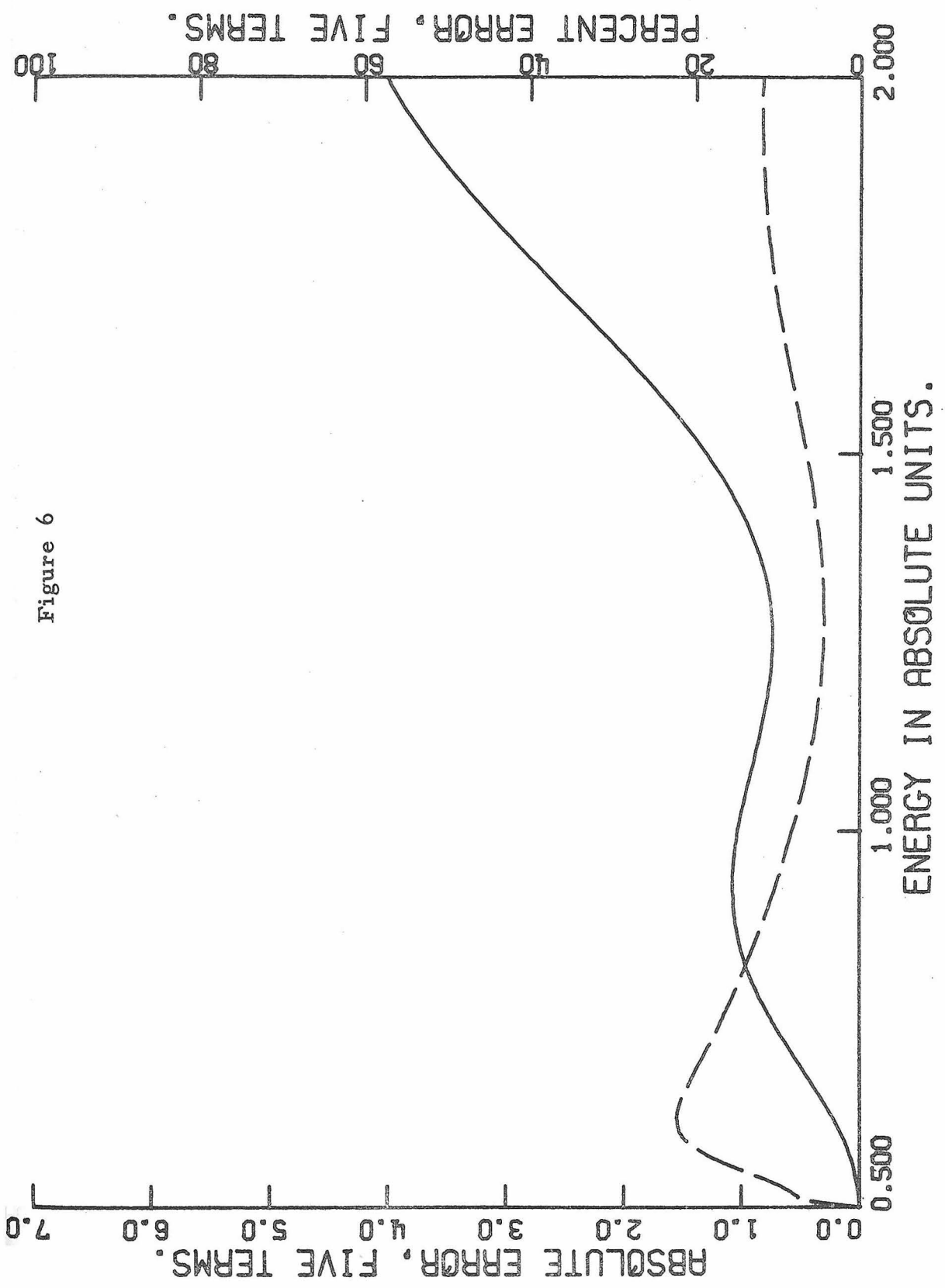
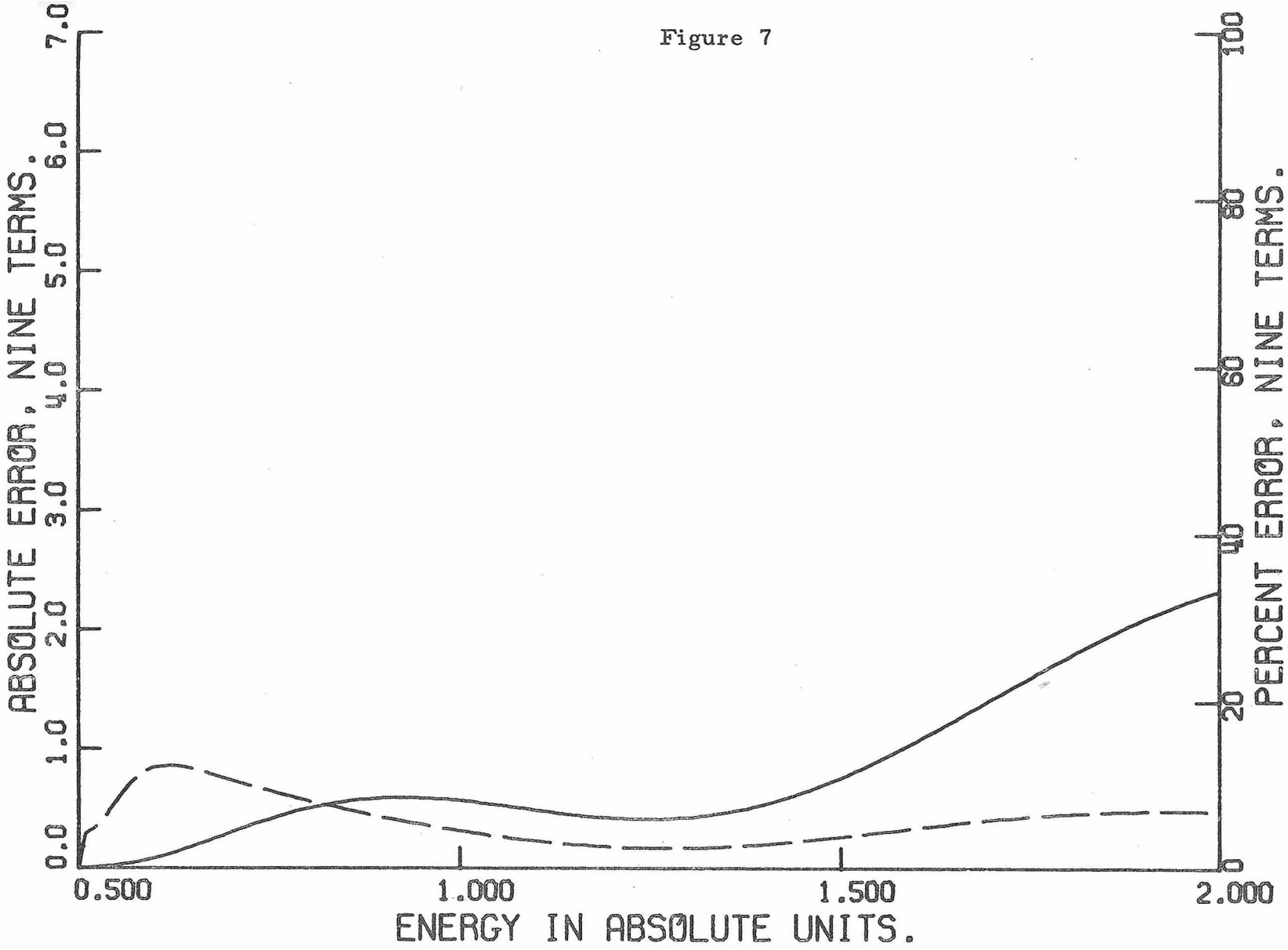

ABSOLUTE ERROR, FIVE TERMS.
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
PERCENT ERROR, FIVE TERMS.
0
20
40
60
80
100
0.500
1.000
1.500
2.000
ENERGY IN ABSOLUTE UNITS.

Figure 6

Figure 7


ABSOLUTE ERROR, NINE TERMS.
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
PERCENT ERROR, NINE TERMS.
0
20
40
60
80
100
0.500
1.000
1.500
2.000
ENERGY IN ABSOLUTE UNITS.

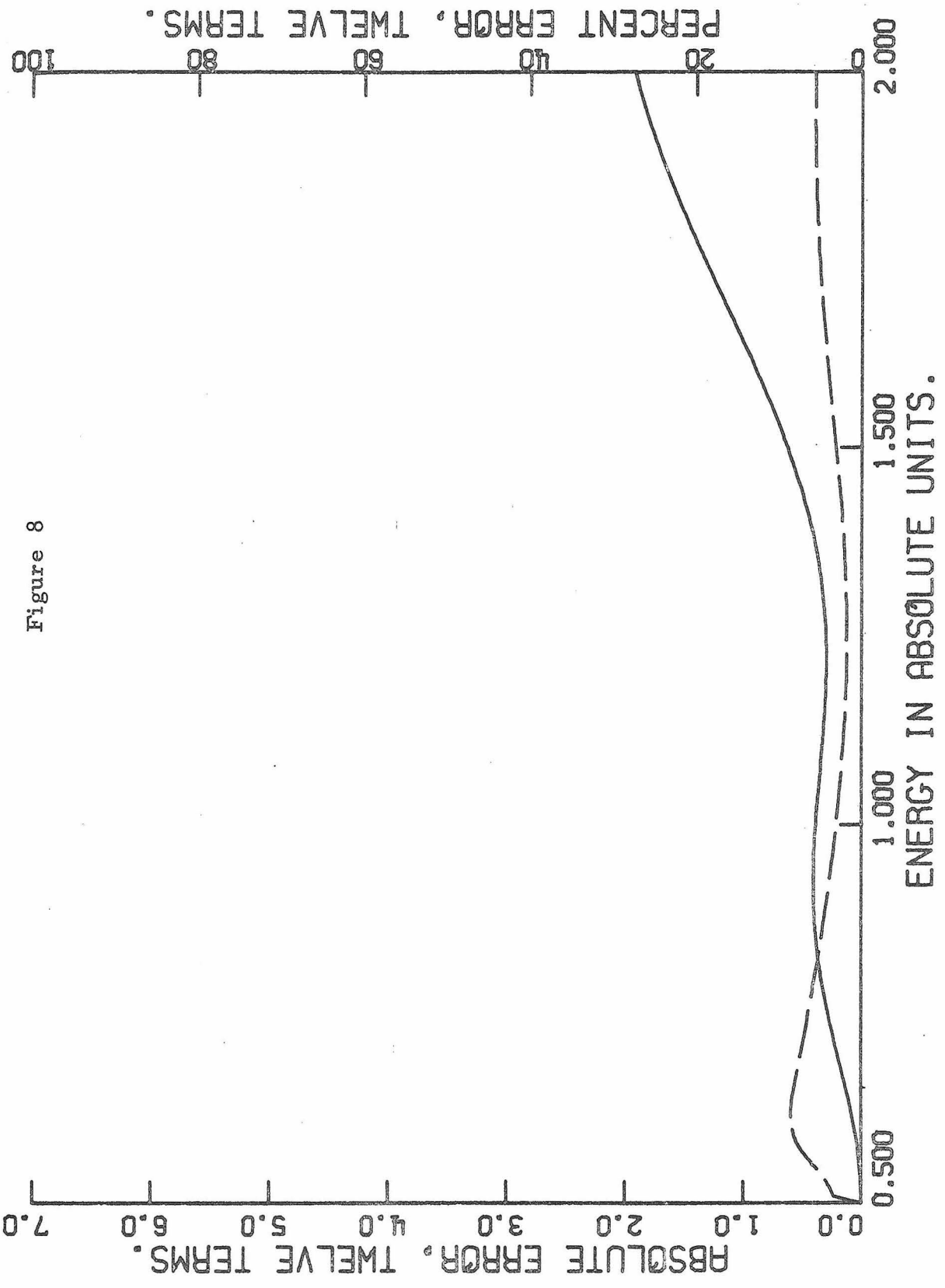

ABSOLUTE ERROR, TWELVE TERMS.
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
PERCENT ERROR, TWELVE TERMS.
0
20
40
60
80
100
0.500
1.000
1.500
2.000
ENERGY IN ABSOLUTE UNITS.

Figure 8

References

Ab68 Milton Abramowitz, Irene A. Stegun, Handbook of Mathematical Functions, Section 25, p. 877, National Bureau of Standards, Applied Mathematics Series, Vol. 55, 7th printing, (1968)

Al67 A. C. Allison, A. Dalgarno, The Rotational Excitation of Molecular Hydrogen, Proceedings of the Physical Society, (London), 90, 609, (1967)

Al72 Millard H. Alexander, Roy G. Gordon, Exact Solutions to the Coupled Hartree-Fock Perturbation Equations, Jour. Chem. Phys., 56, #8, 3823, (1972)

Am66 I. Amirkhanov, V. P. Zhigunov, B. N. Zakhar'ev, Collisions With Particle Redistribution, JINR-P4-2983, 18 pages, (1966), [Russian]

An69 K. G. Anlauf, D. H. Maylotte, J. C. Polanyi, R. B. Bernstein, Rates of Endothermic Reactions for HCl + (I or Cl), Jour. Chem. Phys., 51, 5716, (1969)

Au69 N. Austern, Sasakawa Theory of Reactions, Physical Review, 188, #4, 1595, (1969)

Ba65 L. L. Barnes, N. F. Lane, C. C. Lin, Calculations of Electron Atom Cross Sections, Physical Review, A137, 388, (1965)

Ba71 M. Baer, D. Kouri, Rearrangement Channel Operator Approach to Three Body Scattering, Physical Review A, 4, #5, 1924, (1971)

Ba72a M. Baer, D. J. Kouri, Theory of Reactive Scattering. II Application of the τ Operator Formalism to a Linear Model for Three Body Rearrangements, Jour. Chem. Phys., 56, #10, 4840, (1972)

Ba72b M. Baer, D. J. Kouri, Comment on the Quantum Mechanical Model of Three Body Rearrangement Scattering, Jour. Chem. Phys., 56, #5, 2491, (1972)

Ba73 Michael Baer, Aron Kuppermann, To be Published, (1973)

Be68 Ju. M. Berezanskii, Expansions in Eigenfunctions of Self-adjoint Operators, Chapter 1, Section 3, American Mathematical Society, (1968)

Be71 Charles F. Bender, Peter K. Pearson, Stephen V. O'Neil, Henry F. Schaefer, Potential Energy Surface Including Electron Correlation for the Chemical Reaction $F + H_2 \rightarrow FH + H$, LBL-250 Preprint, October, 1971, Lawrence Berkeley Laboratory

Be72 Charles F. Bender, Stephen V. O'Neil, Peter K. Pearson, Henry F. Schaefer, Potential Energy Surface Including Electron Correlation for the Chemical Reaction $F + H_2 \rightarrow HF + H$, II. Refined Linear Surface, LBL-630 Preprint, March, 1972, Lawrence Berkeley Laboratory

Bo66 Andrew D. Booth, D. Sc., Numerical Methods, p. 164, 3rd Ed., London, Butterworths (1966)

Bo71 Joel Bowman, Aron Kuppermann, Classical and Quantum Reaction Probabilities and Thermal Rate Constants for the

Collinear H_3 Exchange Reaction With Vibrational Excitation, Chem. Phys. Lett., 12, #1, 1, (1971)

Bo73 George C. Schatz, Aron Kuppermann, The Role of Direct and Resonant Processes in the Collinear $H+H_2$ Exchange Reaction, Jour. Chem. Phys., To Be Published.

Br26a T. J. I. Bromwich, An Introduction to the Theory of Infinite Series, pp. 54, 88, 233, Macmillan, (1926)

Br26b T. J. I. Bromwich, An Introduction to the Theory of Infinite Series, pp. 123, 138-139, Macmillan, (1926)

Ca69a Brice Carnahan, H. A. Luther, James O. Wilkes, Applied Numerical Methods, p. 384, John Wiley, (1969)

Ca69b Brice Carnahan, H. A. Luther, James O. Wilkes, Applied Numerical Methods, Chapter 7, Section 7.3, p. 430, John Wiley, (1969)

Co10 P. H. Cowell, A. C. D. Crommelin, The Orbit Elements of Halley's Comet, Astronomische Nachrichten, Band 185, Nr. 4433, 265, (1910)

Co60 Lothar Collatz, Numerical Treatment of Differential Equations; Section V, Boundary Value Problems in Partial Differential Equations; p. 422, 3rd Ed., Springer-Verlag, Berlin, (1960)

Co61a Earl A. Coddington, An Introduction to Ordinary Differential Equations, p. 67, Prentice-Hall, (1961)

Co61b J. W. Cooley, An Improved Eigenvalue Corrector Formula for Solving the Schrödinger Equation for Central Fields,

Mathematics of Computation, 15, 363, (1961)

De59 L. M. Delves, Tertiary and General Order Collisions (I), Nuclear Physics, 9, 391, (1959)

De60 L. M. Delves, Tertiary and General Order Collisions (II), Nuclear Physics, 20, 275, (1960)

Di68a D. J. Diestler, V. McKoy, Quantum-Mechanical Treatment of Inelastic Collisions, I. General Theory and Application to Nonreactive Collisions, Jour. Chem. Phys., 48, #7, 2941, (1968)

Di68b Dennis J. Diestler, Vincent McKoy, Quantum Mechanical Treatment of Inelastic Collisions, II. Exchange Reactions, Jour. Chem. Phys., 48, #7, 2951, (1968)

Di69 Dennis J. Diestler, Coupled Channels Approach to the Quantum Mechanical Treatment of Chemical Exchange Reactions, Jour. Chem. Phys., 50, #11, 4746, (1969)

Di70 D. R. Dion, M. B. Milleur, J. O. Hirschfelder, Quantum Mechanical Model of Three Body Rearrangement Scattering, II. Calculations for a Resonance Energy, Jour. Chem. Phys., 52, #6, 3179, (1970)

Ef67a T. G. Efimenko, V. P. Zhigunov, B. N. Zakhar'ev, The Account of the Pauli Principle in Scattering Theory, JINR-P4-3209, 16 pages, (1967), [Russian]

Ef67b T. F. Efimenko, B. N. Zakhariev, V. P. Zhigunov, Reactions With Rearrangement of Particles, II. Multichannel Coupling Method, JINR-P4-3300, 17 pages, (1967), [Russian]

Ef68a T. G. Efimenko, V. P. Zhagunov, B. N. Zakhariev, Yadernaya Fiziki, 7, #1, 76, (1968), [Russian], English Translation: Reactions With Redistribution of Particles, Soviet Journal of Nuclear Physics, 7, #1, 55, (1968)

Ef68b T. G. Efimenko, B. N. Zakhariev, V. P. Zhigunov, Pauli Principle and Rearrangement Collisions in Unified Theory of Nuclear Reactions, Annals of Physics, (N. Y.), 47, #2, 275, (1968)

Ef68c T. G. Efimenko, Dissertation, Odessa, (1968)

Ef70 T. G. Efimenko, B. N. Zakhariev, O. Khagve, Izv. Akad. Nauk., S.S.S.R., Ser. Fiz., 34, #8, 1798, (1970), [Russian], English Translation: Variational Treatment of Particle Redistribution Reactions, Bull. Acad. Sci., U.S.S.R., Physics Ser., (U.S.A.), 34, #8, 1598, (1970)

Ef71 V. D. Efros, M. V. Zhukov, Elastic N-He^4 Scattering as a Five Body Problem, Phys. Lett., 37B, #1, 18, (1971)

Fi72a Bruce A. Finlayson, The Method of Weighted Residuals and Variation Principles, Section 1.2, p. 7, Vol. 87, Mathematics in Science and Engineering, Academic Press, (1972)

Fi72b Bruce A. Finlayson, The Method of Weighted Residuals and Variation Principles, Section 2.3, p. 24, Vol. 87, Mathematics in Science and Engineering, Academic Press, (1972)

Fo68 L. Fox, I. B. Parker, Chebyshev Polynomials in Numerical Analysis, Oxford University Press, London, (1968)

Go69 R. G. Gordon, A New Method for Constructing Wavefunctions

for Bound States and Scattering, Jour. Chem. Phys., 51, #1, 14, (1969)

Gu70 Vincent P. Gutschick, Vincent McKoy, Dennis J. Diestler, Calculation of Transition Probabilities for Collinear Atom-Diatom and Diatom-Diatom Collisions With Lennard-Jones Interaction, Jour. Chem. Phys., 52, #9, 4807, (1970)

Gu72a Vincent P. Gutschick, Doctoral Thesis, p. 318, California Institute of Technology, (1972)

Gu72b Vincent P. Gutschick, Doctoral Thesis, p. 316, California Institute of Technology, (1972)

Ha23 Jacques Salomon Hadamard, Lectures on Cauchy's Problem in Linear Partial Differential Equations, Yale University Press, (1923)

Ha57 D. R. Hartree, The Calculation of Atomic Structures, p. 71, John Wiley and Sons, New York, (1957)

Ha65 R. W. Hamming, Numerical Methods for Scientists and Engineers, p. 215, McGraw-Hill, (1965)

He70 Anthony C. Hearn, Reduce 2 User's Manual, Stanford Artificial Intelligence Project, Comp. Sci. Dept. Memo AIM-133, Report Stan-CS-70-181, (1970)

Hu43 Hugh M. Hulburt and J. O. Hirschfelder, The Transmission Coefficient in the Theory of Absolute Reaction Rates, Jour. Chem. Phys., 11, #6, 276, (1943)

Ja24 J. Jackson, Note on the Numerical Integration of $\partial^2 x/\partial t^2 = f(x,t)$, Monthly Notices of the Royal Astronomical Society,

84, #8, 602, (1924)

Ka57 Walter Kauzmann, Quantum Chemistry, Chapter 4, Academic Press, (1957)

Ki72 Yasuhiro Kitazoe, Tamotsu Sekiya, An Approach to the Unified Theory of Nuclear Reactions, Progress in Theoretical Physics, 47, #2, 470, (1972)

Kl69 B. Kleinman, K. T. Tang, Comparison of Quantum and Classical Theories of an Idealized Three Body Rearrangement Collision, Jour. Chem, Phys., 51, #10, 4587, (1969)

Kr70 M. Krauss, F. H. Mies, Molecular Orbital Calculation of the Shape Resonance in N_2^-, Physical Review A, 1, #6, 1592, (1970)

La67 Neal F. Lane, S. Geltman, Rotational Excitation of Diatomic Molecules by Slow Electrons, Application to H_2, Physical Review, 160, #1, 53, (1967)

Le65 F. S. Levin, Coupled Equations Method for the Scattering of Identical Particles, Physical Review, 140, #4B, B1099, (1965)

Le66a F. S. Levin, Coupled Equations for Rearrangement Scattering, Physical Review, 141, #3, 858-62, (1966)

Le66b F. S. Levin, Coupled Equations Method for the Scattering of Identical Particles, II, Physical Review, 149, #4, 1212, (1966)

Le68a W. A. Lester, R. B. Bernstein, Computational Procedure for the Close-Coupled Rotational Excitation Problem: Scattering of Diatomic Molecules by Atoms, Jour. Chem. Phys.,

48, #11, 4896, (1968)

Le68b W. A. Lester, De Vogelaere's Method for the Numerical Integration of Second Order Differential Equations Without Explicit First Derivatives: Application to Coupled Equations Arising from the Schrödinger Equation, Jour. Comp. Phys., 3, 322, (1968)

Le68c W. A. Lester, Wisconsin Theoretical Chemistry Institute, Technical Report, Wis-285, (1968)

Lo70 D. J. Locker, D. J. Wilson, Reactive Scattering, A Simple Three Body Model, Jour. Chem. Phys., 53, 2858, (1970)

Ma57 R. Marriott, The Conversion of Metastable Helium from the Singlet to the Triplet State by Electron Collision, Proccedings of the Physical Society of London, 70A, 288, (1957)

Ma59 J. Mazur, Robert J. Rubin, Quantum Mechanical Calculation of the Probability of an Exchange Reaction for Constrained Linear Encounters, Jour. Chem. Phys., 31, #5, 1395, (1959)

Ma64 R. Marriott, Molecular Collision Cross Sections and Vibrational Relaxation in Carbon Monoxide, Proceedings of the Physical Society, (London), 83, 159, (1964)

Me70 R. Meyer, Trigometric Interpolation Method for One-Dimensional Quantum Mechanical Problems, Jour. Chem. Phys., 52, #4, 2053, (1970)

Mi69 William H. Miller, Coupled Equations and the Minimum Principle for Collisions of an Atom and a Diatomic Molecule, Including Rearrangements, p.410, Jour. Chem. Phys., 50, #1, 407, (1969)

Mi71a G. Miller, J. C. Light, Quantum Calculations of Collinear Reactive Triatomic Systems, Jour. Chem. Phys., 54, #4, 1635, (1971)

Mi71b G. Miller, J. C. Light, Quantum Calculations of Collinear Reactive Systems, $H + Cl_2 \rightarrow HCl + Cl$, Jour. Chem. Phys., 54, #4, 1643, (1971)

Mi72 Paulette B. Middleton, Robert E. Wyatt, Broken Path Model of Reactive Collisions: Application to Collinear (H, H_2), Jour. Chem. Phys., 56, #6, 2702, (1972)

Mo62 E. M. Mortensen, K. S. Pitzer, Theoretical Probabilities for Various Isotopic Reactions of the Type $H + H_2 \rightarrow H_2 + H$, p.57, Chemical Society (London), Special Publication #16, The Transition State, (1962)

Mo65a N. F. Mott and H. S. W. Massy, The Theory of Atomic Collisions, p. 388, 3rd Ed., Clarendon Press, (1965)

Mo65b N. F. Mott and H. S. W. Massy, The Theory of Atomic Collisions, Chapter XIII, Section 5.1, P. 371, 3rd Ed., Oxford Clarendon Press, (1965)

Mo65c N. F. Mott and H. S. W. Massy, The Theory of Atomic Collisions, pp. 91, 332, 371, 3rd Ed., Oxford Clarendon Press, (1965)

Mo68 Earl M. Mortensen, Permeabilities and Transmission Coefficients for Various Isotopic Reactions of the Type $H + H_2 \rightarrow H_2 + H^*$, Jour. Chem. Phys., 48, #9, 4029, (1968)

Mu56 D. E. Muller, A Method for Solving Algebraic Equations

Using a Automatic Computer, Mathematical Tables and Other Aids to Computation, 10, 208, (1956)

Na61 National Physics Laboratory, Notes on Applied Science, #16, Modern Computing Methods, p. 88, Department of Scientific and Industrial Research, London, 2nd Ed., (1961)

Nu33 B. Numerov, Publ. de l'Observ. Astrophys., Central Russie, 2, 188, (1933)

Ra69a Philip Rabinowitz, Numerical Methods for Nonlinear Algebraic Equations, p. 115, Gordon and Breach, (1969)

Ra69b Charles C. Rankin, John C. Light, Quantum Solution of Collinear Reactive Systems: $H + Cl_2 \rightarrow HCl + Cl^*$, Jour. Chem. Phys., 51, #5, 1701, (1969)

Re69 Karel Rektorys, Survey of Applicable Mathematics, p. 892, M.I.T. Press, (1969)

Ri68 Merle Eugene Riley, Doctoral Thesis, California Institute of Technology, p. 64, (1968)

Ro70 P. D. Robinson, Quantum Mechanical Model of Three Body Rearrangement Scattering, I. Formal Solution of the Helmholtz Equation on a Square, Jour. Chem. Phys., 52, #6, 3175, (1970)

Ru56 R. A. Rubenstein, M. Huse, S. Machlup, Numerical Solution of the Schrodinger Equation for Central Fields, Mathematical Tables and Other Aids to Computation, 10, 30, (1956)

Sc65 J. B. Scarborough, Differential Equations and Applications, Chapters XIX and XX, Waverly Press, (1965)

Sc70 T. P. Schafer, P. E. Siska, J. M. Parson, F. P. Tully, Y. C. Wong, Y. T. Lee, Crossed Molecular Beam Study of $F + D_2$, Jour. Chem. Phys., 53, 3385, (1970)

Sc73 George Schatz, Joel Bowman, Aron Kuppermann, Jour. Chem. Phys., (In Press), (1973)

Sh68a I. Shavitt, R. M. Stevens, F. L. Minn, M. Karplus, Potential Energy Surface for H_3, Jour. Chem. Phys., 48, #6, 2700, (1968)

Sh68b Isaiah Shavitt, Correlation of Experimental Rate Constants of the Hydrogen Exchange Reaction With a Theoretical H_3 Potential Surface, Using Transition-State Theory, Jour. Chem. Phys., 49, #9, 4048, (1968)

Si66 Yu. A. Simonov, Yad. Fiz. 3, 630, (1966), [Russian], English Translation: The Three Body Problem, A Complete System of Angular Functions, Soviet Journal of Nucl. Phys., 3, 461, (1966)

Sk59 S. Skillman, Efficient Method for Solving Atomic Schrödinger's Equation, Mathematical Tables and Other Aids to Computation, 13, 299, (1959)

Sm65 G. D. Smith, Numerical Solution of Partial Differential Equations, p. 132, Oxford University Press, (1965)

Sm66 Kenneth Smith, R. J. Henery, P. G. Burke, Scattering of Electrons by Atomic Systems With Configurations $2p^q$ and $3p^q$, Physical Review, 147, #1, 21, (1966)

So64 S. L. Sobolev, Partial Differential Equations of Mathema-

tical Physics, p. 382, Addison-Wesley, (1964)

Ta69 K. T. Tang, B. Kleinman, M. Karplus, Solvable Quantum-Mechanical Model of Three-Body Rearrangement Scattering, Jour. Chem. Phys., 50, #3, 1119, (1969)

Ti62 E. C. Titchmarsh, Eigenfunction Expansions Associated With Second Order Differential Equations, Section 1.5, Part 1, 2nd Ed., Clarendon Press, (1962)

Tr26 E. Trefftz, Ein Gegenstuck zum Ritzchen Verfahren, pp. 131-137, Zurich, Sept. 12 to 17, Proceedings of the 2nd International Congress of Applied Mechanics

Tr28 E. Trefftz, Konvergenz und Fehlerschatung beim Ritzschen Verfahren, Mathematischie Annalen, 100, 503, (1928)

Tr70 Donald Gene Truhlar, Doctoral Thesis, p. 214, Part 1, California Institute of Technology, (1970)

Vo55 Rene de Vogelaere, A Method for the Numerical Integration of Differential Equations of Second Order Without Explicit First Derivatives, Jour. of Research of the National Bureau of Standards, 54, #3, 119, (1955)

Wa72 Albert F. Wagner, Doctoral Thesis, California Institute of Technology, p. 44, (1972)

We65a H. F. Weinberger, A First Course in Partial Differential Equations, Chapter 2, p. 29, Blaisdell Publishing Company, (1965)

We65b H. F. Weinberger, Partial Differential Equations, p. 51, Blaisdell Publishing Company, (1965)

We67 A. A. Westenburg, N. DeHaus, Atom-Molecule Kinetics Using E.S.R. Detection, Jour. Chem. Phys., 47,#4, 1393, (1967)

Wi65 J. H. Wilkenson, The Algebraic Eigenvalue Problem, Monographs on Numerical Analysis, Clarendon Press, (1965)

Wo72 George Wolken, William H. Miller, Martin Karplus, Theoretical Studies of $H + H_2$ Rotationally, Inelastic Scattering, Jour. Chem. Phys., 56, #10, 4930, (1972)

Wu62 Ta-You Wu, Takashi Ohmura, Quantum Theory of Scattering, Section A, p. 15, and Section P, p. 309, Prentice Hall, (1962)

Za67 B. N. Zakhar'ev, Izvesta Akad. Nauk., S.S.S.R. Ser. Fiz., 31, #10, 1578, (1967), [Russian], English Translation: Review of Nuclear Theories Taking Channel Coupling into Account, Bull. Acad. Sci., U.S.S.R., Physics Series, (U.S.A.), 31, #10, 1618, (1967)

Za68a B. N. Zakhariev, V. V. Pustovalov, V. D. Efros, Yad. Fiz., 8, #2, 406, (1968), [Russian], English Translation: The Three Body Problem. The K-harmonics Method in Problems Involving the Continuum Spectrum, Soviet Journal of Nuclear Physics, 8, #2, 234, (1969)

Za68b B. N. Zakhariev, V. V. Pustovalov, V. D. Efros, Abstracts of the 18th Annual Conference on Nuclear Spectroscopy, Leningrad, p. 166, (1968)

Za69 B. N. Zakhariev, V. V. Pustovalov, V. D. Efros, Ab-

stracts of the 19th Annual Conference on Nuclear Spectroscopy, p. 188, (1969)

Za70 B. N. Zakhariev, V. P. Permyakov, Yu. I. Fenin, Lower Bounds for the Scattering Parameters, JINR-P4-5332, 14 pages, (1970), [Russian]

Za71 B. N. Zakhariev, O. Lkhagva, S. A. Niyasgulov, Yu. I. Fenin, Bounds on Multichannel Scattering Parameters, Il Nuovo Cimento (Italy), 6A, Ser. 2, N2, 151, (1971)

Zh71 M. V. Zhukov, V. D. Efros, Yadernaya Fiziki, 14, #3, 577, (1971), [Russian], English Translation: Reactions in a System of Serveral Nucleons, Soviet Journal of Nucl. Phys., 14, #3, 322, (1972)

Part III

Propositions

ABSTRACT OF PROPOSITION ONE

A bifunctionate method for solving the collinear, three atom Schrödinger equation proposed by Diestler in 1969 is wrong. The method fails because the closed coupled equations it solves possess eigenfunction decay points within the interaction region. A bifunctionate method is proposed which will correctly solve the equations for reactive scattering.

Proposition: The bifunctionate solution method for solving the collinear, three atom Schrödinger equation published by Diestler (Di69) is wrong. The method introduces sperious nodes into the reactive scattering wavefunction. A correct bifunctionate method is proposed. This method requires solution part recombination at a sectioning line.

In 1969, Dennis J. Diestler (Di69) proposed a method for solving the collinear, three atom Schrödinger equation for energies below the three particle threshold. This method was based on a proposal to create the scattering solution in two parts, each part of the total solution constructed by an expansion in asymptotic eigenfunctions. This formalism for solving the second order partial differential equations of scattering is wrong.

A brief outline of Diestler's proposals will be presented before the deficiencies in this formalism are described. The collinear collision equations will be posed in the (x_{12}, x_{23}) coordinate scheme previously used in reactive scattering studies (Di68a, Di68b, Tr70). As has been done previously, these coordinates will be assumed orthoginal.

In figure 1.1, a typical potential surface for the reactive, collinear encounter is shown with several important coordinate lines added. The lines ℓ_{12} and ℓ_{23} denote the lines of decay of the bound state asymptotic eigenfunctions in the x_{12} channel and

and the x_{23} channel, respectively. At the lines of decay, all of the functions of the discrete eigenfunction set can be taken to be zero. The terminology x_{12} channel and x_{23} channel will be used to denote regions of the potential surface where x_{ij} describes the free atom position in the three atom system.

Diestler's paper describes a method for preparing the total solution to the scattering equations by the Method of Weighted Residuals (Fi72). The novel feature of Diestler's idea is contained in the manner in which he proposes to create the primative solutions that are later linearly combined to meet the boundary conditions. Each primative in this approach to the final solution, is created in two related parts. The first part of the solution is constructed by solving the close-coupled equations obtained by expanding part 1 of the complete primative in the asymptotic eigenfunctions of one channel. One half of the total primative is thus represented by a sum of products of single variable functions.

If it is assumed for the sake of clarity, that the first part of the primative was created in the x_{23} channel, then this solution segment will die out beyoud the line ℓ_{23}. This behavior is incorporated into the total mechanism for solving the partial differential equation by using the line ℓ_{23} as a limit point for an expansion of the second part of the primative solution.

The second part of the primative is also created by an expansion in asymptotic eigenfunctions but in this case, the ex-

pansion set is the set of oscillator eigenfunctions of the remaining channel. This would be the x_{12} channel asymptotic eigenfunctions under the expansion convention just adopted. The second part of the single, full solution being created is related to the first part of this same solution by matching the two series expansions in value and derivative at the line ℓ_{23}.

The close-coupled equations which can be obtained from the Schrödinger equation and the eigenfunction expansion of part two must be solved before the part two solution is complete. The closed coupled equations for the expansion coefficients were to be solved by a propagator method of arbitary type. Diestler indicated that the x_{23} channel equations should be solved from the zero value of the x_{23} coordinate while the x_{12} channel equations were to be propagated in value and derivative from the line, ℓ_{23}.

Once one primative was developed by Diestler's technique, the process was repeated to create a set of such primatives. These primatives were then to be linearly combined to solve the complete scattering equations by use of the Method of Weighted Residuals.

The Flaw in This Formalism:

The invalidating feature of Diestler's method appears in the method by which the primatives of his formalism are created. If these primatives were valid solutions to the partial differential equation, then the linear combination of the primative set by the Method of Weighted Residuals would yield a correct complete

scattering solution. As will be shown shortly, each primative this technique creates is not a solution to the differential relationship and it is for this reason that the method fails.

Since each primative solution is here asserted to be invalid, all features of the primative combination procedure and all aspects of the linear independence of the primative set can be ignored, This study will concentrate on the construction of one primative using the regime prescribed in De69.

The two part Diestler solution will be denoted $\Phi_1(x_{12}, x_{23}) + \Phi_2(x_{12}, x_{23})$. The channel specificity already presented in the description of Diestler's method will be used for this discussion of the failure of this formalism. Thus, $\Phi_1(x_{12}, x_{23})$ is expanded in the eigenfunction set $\{\phi_j(x_{12})\}$ and $\Phi_2(x_{12}, x_{23})$ is created in the set of $\{\bar{\phi}_k(x_{23})\}$ functions. The equations for these two functions are

$$\Phi_1(x_{12}, x_{23}) = \sum_{i=1}^{N} f_i(x_{23})\,\phi_i(x_{12})$$

and

$$\Phi_2(x_{12}, x_{23}) = \sum_{j=1}^{N} g_j(x_{12})\,\bar{\phi}_j(x_{23}).$$

The function $\Phi_1(x_{12}, x_{23})$ spans the x_{23} channel from $x_{23} = 0$ to $x_{23} = x_{23}^{\circ}$, an asymptotic value. The function $\Phi_2(x_{12}, x_{23})$ continues the primative from ℓ_{23} to x_{12}°, an x_{12} channel asymptotic value.

It now becomes imperative to consider what happens to $\Phi_1(x_{12}, x_{23})$ as $x_{12} \rightarrow \ell_{23}$. At this line, the function $\Phi_1(x_{12}, x_{23})$

goes to zero. However, the reason that $\Phi_1(x_{12}, x_{23})$ has a node at ℓ_{23} is not evident from the potential surface, differential equation or boundary conditions of the scattering equations. The cause of $\Phi_1(x_{12}, x_{23})$'s node is independent of all of these features of the scattering problem. The node appears solely because this part of the primative solution was expanded in asymptotic eigenfunctions of the x_{23} channel.

As the line ℓ_{23} is approached, the eigenfunctions of this expansion decay to zero. Thus, the representation of the primative is failing at the line ℓ_{23} and a node appears in this function solely because the incorrect expansion set has been used to construct $\Phi_1(x_{12}, x_{23})$. This error is compounded by the continuation of the primative from the line ℓ_{23}.

The node at ℓ_{23} is taken as a correct component of the primative when the second part of the solution is calculated. Thus the failure of the eigenfunction representation of a true solution to the scattering equation is continued by the connection process proposed for the two primative parts.

An Analytic Calculation:

A proof of the failure of the Diestler method can be constructed from the uniqueness principle for elliptic partial differential equations. This analysis is based on the work of E. Hopf (Ho27, Be64) who showed that elliptic, partial differential, boundary value problems have unique solutions.

Consider the surface of Figure 1.2. Here the infinite po-

tential surrounding the reacted channel makes the asymptotic regions of both channels square wells. An infinite central mass has been assumed for this collision model so the coordinates x and y are orthoginal. The width of the two equivalent channels is denoted by ℓ and the magnitude of ℓ is such that ℓ is less than the interaction region limits, x° and y°.

The Schrödinger equation in the mass scaled coordinates

$$y = -m_1^{-\frac{1}{2}} x_{12}, \quad x = m_3^{-\frac{1}{2}} x_{23} \tag{1}$$

is

$$\left[\partial^2/\partial y^2 + \partial^2/\partial x^2 - 2/\hbar^2 (V_{123} - E) \right] \Psi = 0 \tag{2}$$

where the interaction potential, V_{123}, will be taken to be a constant. Use the coordinate transform

$$r = \left[(x - x_0)^2 + (y - y_0)^2 \right]^{\frac{1}{2}} \tag{3a}$$

$$\theta = \tan^{-1}\left([x - x_0] / [y - y_0] \right), \tag{3b}$$

to pose the Schrödinger equation as

$$\left[r^{-1} \partial/\partial r (r \partial/\partial r) + \frac{1}{r^2} \partial^2/\partial\theta^2 - 2/\hbar^2 (V_{123} - E) \right] \Psi = 0 \tag{4}$$

This equation will be solved by separation of variables with the separation constant labled λ. Define the constant

$$z_1 = -2/\hbar^2 (V_{123} - E)$$

so that the differential relationship becomes

$$\left[r^2 \partial^2/\partial r^2 R(r) + r \partial/\partial r R(r) + r^2 (z_1 - \lambda/r^2) R(r) \right] = 0 \tag{5a}$$

$$\left[\partial^2/\partial\theta^2 + \lambda \right] T(\theta) = 0 \tag{5b}$$

where

$$\Psi(r, \theta) = R(r)\,T(\theta). \tag{5c}$$

Apply the coordinate scaling $r' = z_1^{\frac{1}{2}} r$ to equation 5a) to obtain the set of equations

$$\left[r'^2 \partial^2/\partial r'^2 + r' \partial/\partial r' + r'^2 (1 - \lambda/r'^2) \right] R(r') = 0, \tag{6a}$$

$$\left[\partial^2/\partial\theta^2 + \lambda \right] T(\theta) = 0. \tag{6b}$$

These are Bessel's equation (Gr31) and the free wave equation (Ab64), respectively. The solutions of these equations are

$$\{ J_\nu(r'),\ Y_\nu(r') \}$$

and

$$\{ \sin(k\theta),\ \cos(k\theta) \},$$

where

$$k^2 = \lambda$$

and

$$\nu^2 = \lambda.$$

The value of λ will be taken to be 1. Also, the irregular Bessel function will be elminated from the solution set and a solution to equation 6) will be taken to be

$$\Psi(r, \theta) = J_1(r')\{ \sin(\theta) + \cos(\theta) \}. \tag{7}$$

By the boundary conditions at r_1 and r_2, it must occur that $z_1^{\frac{1}{2}} r_1$ and $z_1^{\frac{1}{2}} r_2$ are zeroes of the Bessel function. These zeroes will be taken to be the first two sequential zeroes of the regular Bessel function. Hence,

$$z_1^{\frac{1}{2}} r_1 = 3.83171 \tag{8a}$$

and

$$z_1^{\frac{1}{2}} r_2 = 7.01559. \tag{8b}$$

Equation 8) defines the values of E and V_{123}.

With the solution of equation 7) established, let the full Schrödinger problem be rewritten

$$\left[\partial^2/\partial y^2 + \partial^2/\partial x^2 - 2/\hbar^2 (V_{123} - E) \right] \Psi = 0, \tag{9a}$$

$$\Psi(r_1, \theta) = 0 = \Psi(r_2, \theta), \tag{9b}$$

$$\Psi(x_0, y_0) = J_1(x_0 z_1^{\frac{1}{2}}) \cos(0), \tag{9c}$$

$$\Psi(x, y_0) = J_1(y_0 z_1^{\frac{1}{2}}) \sin(\pi/2). \tag{9d}$$

Equation 9) defines one unique solution to the elliptic partial differential equation, namely the function in equation 7). With this unique solution established, the numerical form of this solution will be prepared using the Diestler method.

The asymptotic eigenfunctions $\{ \phi_j(y) \}$ and $\{ \overline{\phi}_k(x) \}$ are square well functions. These functions thus form two infinite, denumerable, complete sets. The solution to the scattering problem of equation 9) can be expanded in a uniformly convergent, variable coefficient series of these functions.

The first part of the Diestler solution will be developed in the x direction. Therefore,

$$\Phi_1(x, y) = \sum_{i=1}^{\infty} f_i(x) \phi_i(y) \tag{10}$$

The boundary conditions on $\Phi_1(x, y)$ are that at x_3,

$$x_3 = (r_2^2 - \ell^2)^{\frac{1}{2}},$$

$$\Phi_1(x_3, y) = 0 \tag{11a}$$

and at $x = x_0$,

$$\Phi_1(x_0, y) = J_1(r') \cos(0). \tag{11b}$$

By inserting the expansion of equation 10) into equation 9a), a set of closed coupled equations for the $f_j(x)$'s is generated. These equations are

$$\left[{}^{\partial^2}/_{\partial x^2} f_m(x) + {}^{2}/_{\hbar^2}(E + \epsilon_m) f_m(x) - {}^{2}/_{\hbar^2} \sum_{i=1}^{\infty} \int \phi_m(y) V_{123} \phi_i(y)\, dy\, f_i(x) \right]$$

$$= 0, \qquad m = 1 \text{ to } \infty. \tag{12}$$

Equation 12) will be solved by the Numerov method with the boundary conditions of equation 11) to determine the set of expansion coefficients $\{ f_m(x) \}$.

The expansion for $\Phi_2(x, y)$ must now be continued from the line $y = \ell$. The expansion for the second part of the function is

$$\Phi_2(x, y) = \sum_{j=1}^{\infty} g_j(y)\, \bar{\phi}_j(x)$$

Since the expansion for $\Phi_1(x, y)$ goes to zero at $y = \ell$, the boundary conditions on $\Phi_2(x, y)$ are

$$\Phi_2(x, \ell) = 0 \tag{13a}$$

and

$$\Phi_2(x, y_0) = J_1(r') \sin(\pi/2) \tag{13b}$$

The closed coupled equations for the expansion coefficients, $g_j(y)$, are

$$\left[{}^{\partial^2}/_{\partial y^2} g_k(y) + {}^{2}/_{\hbar^2}(E + \epsilon_k) g_k(y) - {}^{2}/_{\hbar^2} \sum_{j=1}^{\infty} \int \phi_k(x) V_{123} \phi_j(x)\, dx\, g_j(y) \right]$$

$$= 0, \qquad k = 1 \text{ to } \infty. \qquad (14)$$

Again, equation 14) with the boundary conditions of equation 13) will be solved by Numerov propagation. This completes the solution by Diestler's technique.

The two solutions, Ψ and $\Phi_1 + \Phi_2$ should be equal because they meet the same boundary conditions and satisfy the same differential equation. However, the function Ψ has no zeroes in the interaction region. There are no nodal lines for this function anywhere within the finite potential area.

The Diestler solution $\Phi_1 + \Phi_2$, has a node at the line $y = \ell$. The two solutions are therefore not equivalent. Hence, by the uniqueness property of the elliptic partial differential equation, one of these solutions must be wrong.

The erronious solution is the eigenfunction expansion solution created by Diestler's method, thus showing that the asymptotic expansion method Diestler proposed is wrong.

Q. E. D.

Validating Adjustments for a Bifunctionate Method

While the two part solution prepared by Diestler is invalid, a two segment solution can be proposed that will solve the reactive Schrödinger equation. The two parts of the final primitive will be channel specific for the collinear potential surface of Figure 1.1.

The two halves of the final primitive will be generated in the same way so the generation technique will be detailed for

only one part of the total solution. Let the primitive wavefunction be $\Psi = c_1 \Phi_1 + c_2 \Phi_2$. The function Φ_1 will be generated in the entrance channel from the asymptotic line x_{23}° to the sectioning line $x_{23} = x_{12}$. The solution must be created by a Cauchy technique from value and derivative data specified at $x_{23} = x_{23}^{\circ}$ or must be generated such that Cauchy data can be evaluated at the sectioning line $x_{23} = x_{12}$. Thus, the means of generating Φ_1 can be certain of the numerical methods described in section 3 of Part II of this thesis.

A coupled channels integration will ordinarily not be a possible means of solving for the solution parts Φ_1 and Φ_2. The partial differential equation will normally have to be solved without eigenfunction expansion techniques in the quadrilateral region bounded by the entrance channel, x_{23}° and the sectioning line.

Once the two sets of primitive halves, Φ_1 and Φ_2, have been generated, the two sets are recombined into one set of complete primitives by matching the two sets of functions in value and derivative at the sectioning line $x_{23} = x_{12}$. This matching process is accomplished with a set of constant multipliers which multiply the two matrices, Φ_1 and Φ_2. Upon specifing the constants which appear in the matching condition equations, a full set of primitives is ready to be manipulated to the standard scattering boundary conditions.

The asymptotic boundary conditions for the reactive scattering problem will be met by the use of the Method of Weighted Resid-

uals. This recombination process operates on the complete primitive set just composed from the two partial primitive sets.

The two part solution method has been used by Smith and Burke (Sm61) to iteratively solve the integro-differential equations of electron scattering. It can equally well be applied to the three atom reactive scattering problem to solve the Schrödinger equation. Such an application should give a convergent, bifunctionate solution method for quantum, reactive encounters.

1: Figure Captions

Figure 1.1: A typical potential surface for a three atom, collinear collision is contour plotted in this figure. The lines of decay for the asymptotic eigenfunctions of the entrance and reacted channel, labeled ℓ_{23} and ℓ_{12} respectively, are shown in the plot.

Figure 1.2: The potential surface for the system treated with Diestler's Bifunctionate Solution Method. The value of the potential outside the channel is infinity.

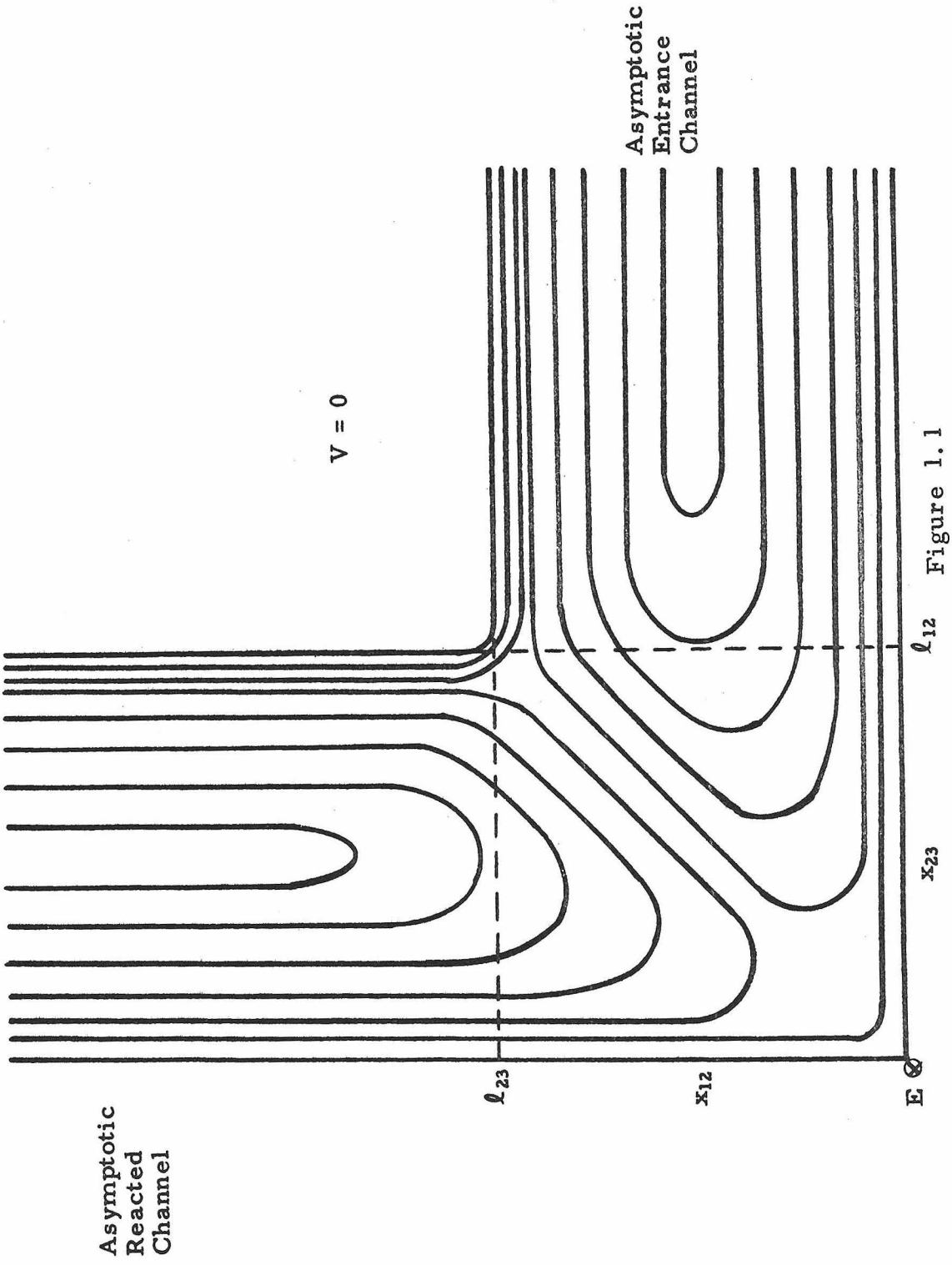

Asymptotic
Reacted
Channel
V = 0
Asymptotic
Entrance
Channel
ℓ_{23}
x_{12}
E
x_{23}
ℓ_{12}

Figure 1.1

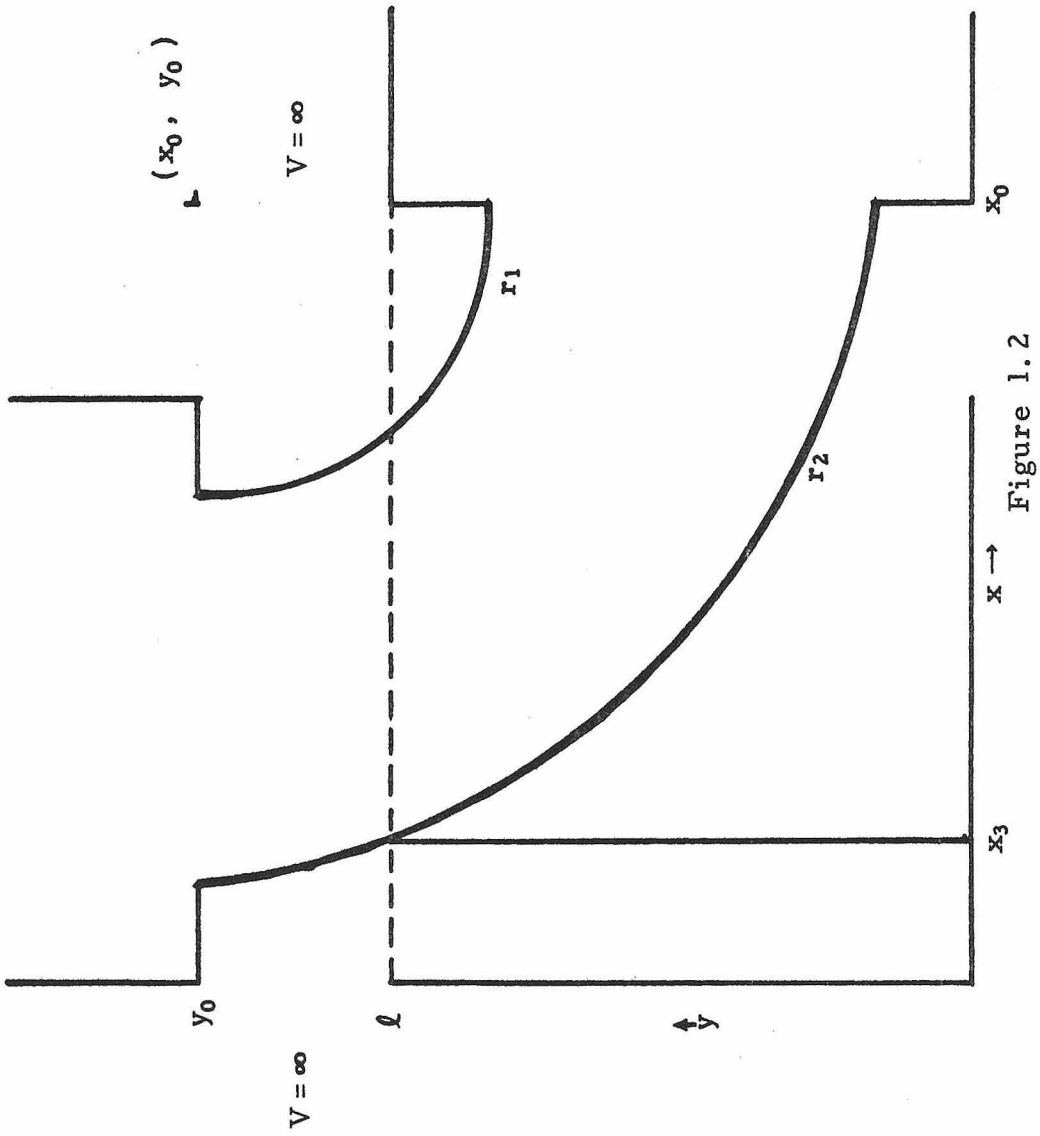

(x_0, y_0)
$V = \infty$
r_1
r_2
x_0
x_3
y_0
ℓ
$x \rightarrow$
$\leftarrow y$
$V = \infty$

Figure 1.2

1: References

Ab64 Milton Abramowitz, Irene A. Stegun, Handbook of Mathematical Functions, pages 69 and 77, National Bureau of Standards, Applied Mathematics Series, Vol. 55, (1964)

Be64 Lipman Bers, Fritz John, Martin Schechter, Partial Differential Equations, p. 283, Vol. 3, Lectures in Applied Mathematics, Interscience Publishers, (1964)

Di68a D. J. Diestler, V. McKoy, Quantum Mechanical Treatment of Inelastic Collisions. I. General Theory and Application to Non-reactive Collisions, Jour. Chem. Phys., 48, #7, 2941, (1968)

Di68b D. J. Diestler, V. McKoy, Quantum Mechanical Treatment of Inelastic Collisions. II. Exchange Reactions, Jour. Chem Phys., 48, #7, 2951, (1968)

Di69 D. J. Diestler, Coupled Channels Approach to the Quantum Mechanical Treatment of Chemical Exchange Reactions, Jour. Chem. Phys., 50, #11, 4746, (1969)

Fi72 Bruce A. Finlayson, The Method of Weighted Residuals and Variation Principles, section 1.2, p. 7, Vol. 87, Mathematics in Science and Engineering, Academic Press, (1972)

Gr31 Gray, Mathews and MacRobert, Treatise of Bessel Functions, p. 7, equation 7, Macmillian and Co., London, (1931)

Ho27 E. Hopf, Elementare Bemerkungen über die Lösungen partieller Differential gleichungen zweiter Ordnung Vom elliptischen Typus, pages 147 to 152, Sitber Preuss. Akad. Wiss., Berlin, Vol. 19, (1927)

Tr70 Donald Gene Truhlar, Doctoral Thesis, part 1, p. 214, California Institute of Technology, (1970)

Sm61 Kenneth Smith, P. G. Burke, Effect of Virtual Excitations on the Elastic Scattering of Electrons and Positrons by Atomic Hydrogen, Physical Review, 123, #1, 174, (1961)

ABSTRACT OF PROPOSITION TWO

The compound 1, 1-bis (4-chlorophenyl)-2, 2, 2- Trichloro-ethane, commonly called D. D. T., has been shown to stimulate the breakdown of estrogenic and androgenic steroids in certain species of the animal classes Aves and Mammalia. D. D. T. will cause steroid imbalance in humans and, at certain periods of development, permenant damage will result from exposure to D. D. T.

Proposition: 1,1-bis(4 chlorophenyl)-2,2,2-Trichloroethane, commonly called D. D. T., will cause metabolic upsets in the developing male human fetus by accellerating the decomposition of and inhibiting the capacity to store, androgenic hormones.

Over the past 15 years, it has become apparent that many species of preditory birds and game fowl were undergoing catastrophic reductions in their populations (1-5). A few of the birds involved were the Bermuda Petel (Pterodroma cahow) (6), the American Woodcock (Philohela minor) (2), the Peregrine Falcon (Falco peregrinus) (7), the Bald Eagle (Haliaeetus leucocephalus) (8), and the Golden Eagle (Aquila chrysaetaes) (9). On the basis of isolation of their habitat and breeding grounds or because of legal protection, these population declines did not appear to be directly related to the hostile actions of man.

Investigations traced the population declines back to a lack of breeding success caused by nesting failures in the afflicted species. As the cause of this nesting failure was sought, it became apparent that starting in 1946 there had been a sudden sharp drop in the calcium content and hence the structural capacities of the egg shells of the affected birds. The D. D. T. content of the eggs and parent birds was, in all cases, high (1-12). Further studies showed that there existed a correlation between the concentration of D. D. T. or its metabolites in th viable young or

eggs of the affected species and the rate of reproduction failure (13, 14). It was also demonstrated that there was a correlation between the incidence of breeding failure in some of the affected birds and the amount of D.D.T. expended in their local environment in a given year (2).

This statistical information lead to controlled feeding experiments in which D.D.T. and D.D.E. in concentrations of 3 parts per million induced eggs with 13.5% thinner shells which broke 6 times as often and produced less than half as many healthy offspring when compared to controls (15, 16, 17). These findings as well as the observed behavior of the birds themselves (18), all indicated an disruption of the calcium metabolism of the endangered species. This metabolic upset was caused by D.D.T.

Attempts were now made to determine how D.D.T. altered calcium metabolism. Examination of the route of calcium through the bodies of most birds showed that the steriod hormone estrogen (17β estradiol) was instrumental in controlling the retention of calcium and its incorporation into the egg. This fact and the discovery (19) that p,p' D.D.T. induced a delay in ovulation in the Bengalese Finch (Lonchura stritata), apparently by affecting hormone balance, lead to studies by Peakall (20) which showed that D.D.T. induced hepatic (liver) enzymes in pigeons which broke down the hormone estrogen.

Once the causual process by which D.D.T. promoted population declines in the class Aves was understood, similar effects

were rapidly discovered in other species. In 1967, Walsh, Levin and Conney (21) showed that hepatic enzyme induction by D.D.T. also took place in rats. D.D.T. has been shown to produce the same biological phenomena in male beagle dogs (22).

On the basis of this data, it was proposed (23) that D.D.T. would produce biological disruptions in humans by inducing androgenic and estrogenic steriod imbalance.

This imbalance would result from distuptions in the pathway:

chlosterol → bile acids → corticoids → androgens → estrogens

which occurs in cattle, rats, man and other mammals. By hepatic enzyme induction, D.D.T. would cause a concentration change in one of the compounds of the synthesis chain:

progestosterone → 17αhydroxyprogesterone → Δ^4androstene-3,17dione → 17β hydroxyandrost-4-en-3-one.

This proposal was verified by the development of impotence in farmworkers caused by exposure to D.D.T. (24). While this particular result of enzyme induction by D.D.T. is obviously neither desirable nor appreciated by those parties afflicted, it is not the worst biological effect that can be expected.

Upon discontinuing exposure to all pesticides and administration of methyl testosterone (methyl 17β hydroxyandrost-4-en-3-one) Espir et al (24) found that normal sexual function returned to all those who had been adversely influenced by the pesticide. Such reversable effects are not expected at all stages of human devel-

opment.

For the human fetus or the young child, the disruption of normal hormone balance will, in all probability, result in permenant and irreversable damage to the developing individual. The embryo will receive a significant exposure to D. D. T. through the mother's circulatory system. This exposure will be inhanced by the uterotropic action of D. D. T. (25). The nursing baby will receive a level of D. D. T. two to four times federal pesticide residue limits from his mother's milk (26, 27, 28). The total effects of these exposures will depend on the magnitude of the amount of D. D. T. consumed.

To accertain what biological effects D. D. T. might have on a human fetus, studies should be undertaken on a small population of rats. However, only one half of the rat population, the male fraction, would be used to define D. D. T. induced anomalies.

At the present time, studies on the effects of D. D. T. on estrogen levels in rats, mice and humans indicate that this chlorinated hydrocarbon induces a variety of responces in the blood stream concentration of this steroid. Because D. D. T. does not initiate a predictable process of biological events when influencing estrogen levels and because of the complexity of estrogen related events which do occur when D. D. T. is introduced into an organism, studies of the steroid concentrations of females will not be undertaken. Instead, the behavior of testosterone levels in males under the influence of D. D. T. will be studied.

D.D.T. has a straight forward effect on ambiant blood concentration of testosterone. By inducing the hepatic enzyme testosterone hydroxylase, D.D.T. causes testosterone to be decomposed by the liver at a faster than normal rate. This causes a drop in testosterone concentration in the blood.

It could be argued that significant biological effects will not be found in this study because of the feedback loop nature of most biological systems. Viewing the concentration of testosterone in the blood as one component of a feedback system indicates that the lowering of testosterone levels in the blood will initiate a release of more testosterone, thus righting the hormone balance. This process actually occurs in the mature human and it is probabily partially responsible for the fact that D.D.T. effects in the mature male have been found to be only temporary (24).

In the fetus, however, a significant backup supply of testosterone is not available. Worse yet, D.D.T. has been shown to reduce vitamin A levels in the liver. Vitamin A plays a key role in maintaining the seretory integrity of prostatic epithelial cells (29). By removing the prostate gland as a storage unit for testosterone, D.D.T. would completely immobilize any feedback loop adjustments to ambiant steroid blood concentration.

A wide variety of results are expected from the lowered testosterone levels in a male fetus. D.D.T. has already been shown to produce striking inhibition of testicular growth in cockerels (30) and it is anticipated that delayed or inhibited testicular

growth will be encountered in the fetii of mothers given a diet tainted with D. D. T.

D. D. T. is also expected to interfere with the development of the prostate gland and to cause cirrhosis phenomena in the liver. By influencing the body's supply of vitamin A, D. D. T. may cause eye damage and poor vision.

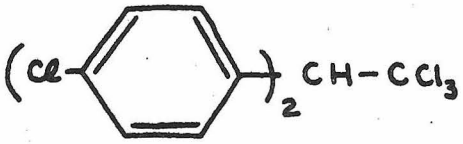
Finally, because a definate timetable of development exists for most mammals, D. D. T. may cause biological sequence problems in offspring chronically exposed to this chemical. By inhibiting changes in hormone concentrations or restricting the development of the glands important in producing or maintaining these hormone concentrations, 1, 1-bis (4 chlorophenyl)-2, 2, 2 Trichloroethane may significantly alter the normal maturation of a chronically exposed individual.

To prove the causual relations asserted above, a chronic exposure study will be done on a bifurcated colony of rats consisting of exposed and control groups. The experimental procedure will follow that of Phillips et al (29) with organ studies performed as described in (23). The anticipated organ metabolites are 7α,6β, and 16α hydroxytestosterone, Δ^{16} androsten-3α-ol, 17α hydroxy-5α-androst-1-en-3-one, androsterone, epiandrosterone, 17β hydroxy-5α-androstan-3-one, 5α androstan-3α-17β diol and their accompanying side products. The sacraficed animals will be drawn from the male fraction of an 120 rat colony, a colony size needed to insure a 95% certainty level in any bio-

logical differences found.

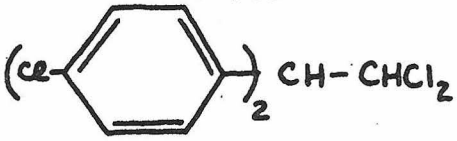
Female rats in the colony will be sacrificed as necessary to conduct fetal studies of D. D. T. effects occurring during gestation. The total time needed to obtain conclusive results from this investigation will vary from a year to a year and a half, depending on the outcome of the initial experiments.

2:List of Formulas



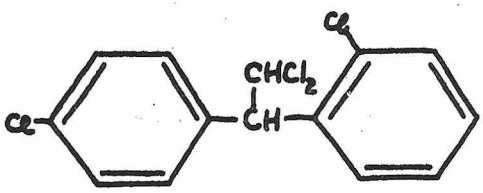
1,1-bis (4-chlorophenyl)-2,2,2-Trichloroethane

Synonyms: DDT; p,p′ DDT



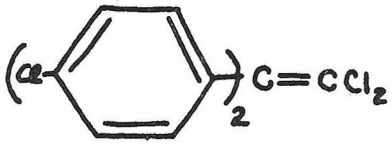
1,1-bis(4-chlorophenyl)-2,2-dichloroethane

Synonyms: DDD; p,p′ DDD



1-(4-Chlorophenyl), 1-(2-Chlorophenyl), 2,2-dichlorethane

Synonym: o,p′ DDD

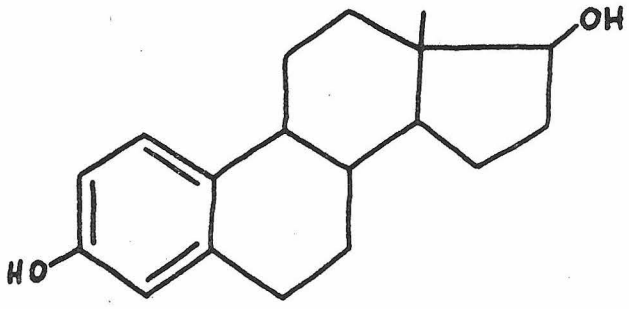


2,2-bis(4-chlorophenyl)-1, 1-dichloroethene

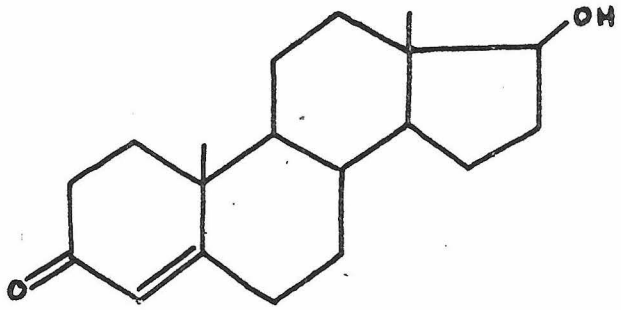
Synonym: DDE

17β estradiol

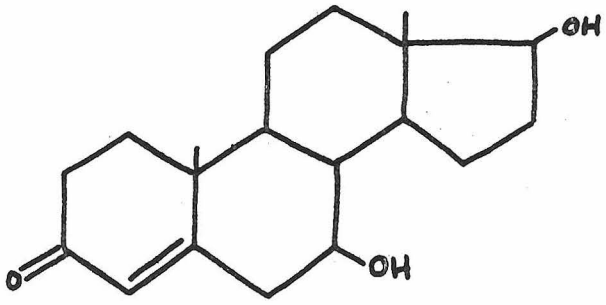
Synonym: Estrogen



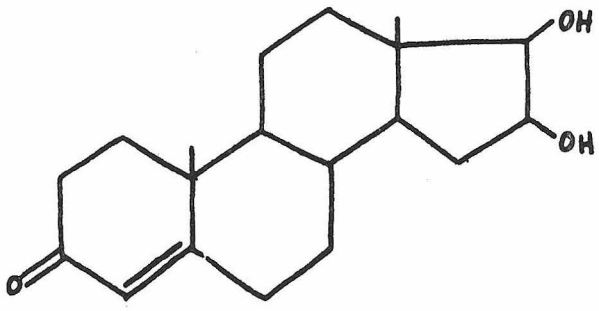
17β hydroxy androst-4-en-3-one
Synonym: Testosterone



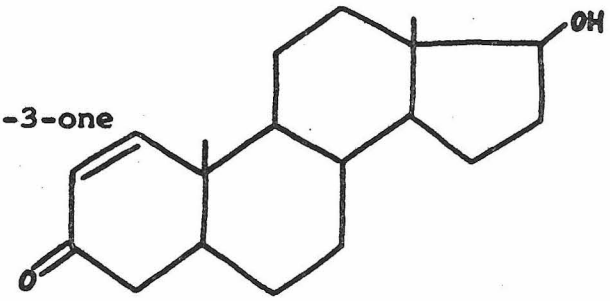
7α, 17β dehydroxy androst-4-en-3-one
Synonym: 7α hydroxytestosterone



16α, 17β dehydroxyandrost-4-en-3-one
Synonym: 16α hydroxytestosterone

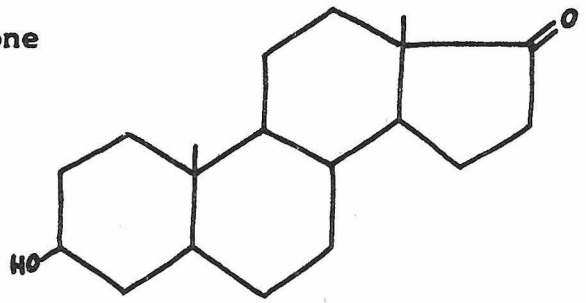


17α hydroxy-5α-androst-1-en-3-one

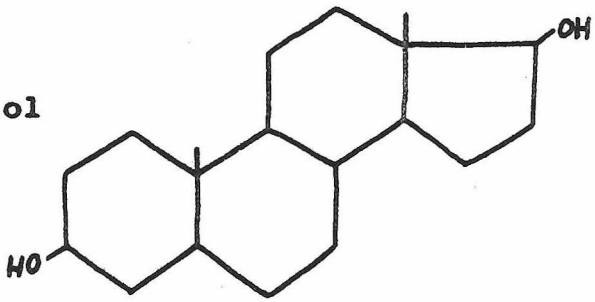


3β hydroxyandrostan-17-one

Synonym: Epiandrosterone

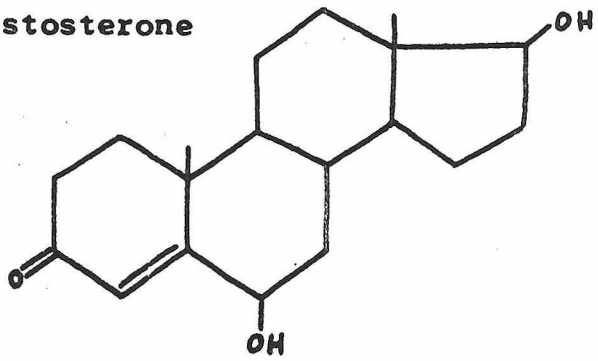


5α androstan-3α, 17β diol

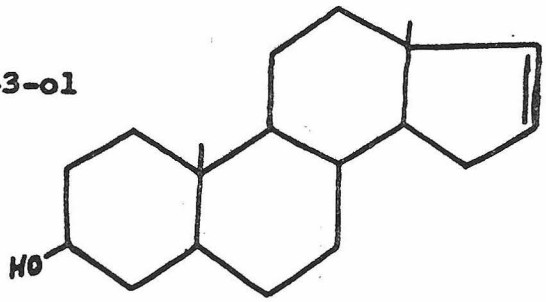


6β, 17β dehydroxyandrost-4-en-3-one

Synonym: 6β hydroxytestosterone

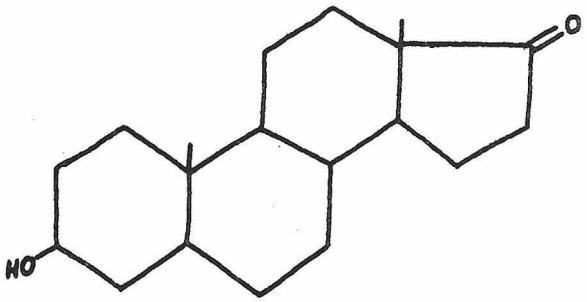


androst-16-en-3-ol

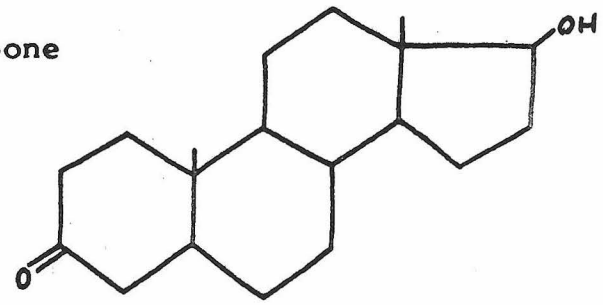


3α hydroxyandrostan-17-one

Synonym: Androsterone



17β hydroxy-5α androstan-3-one



2. References

1. C. F. Wurster, First Rochester Conference on Toxicity, University of Rochester, June 4-6, 1968
2. B. S. Wright, J. Widl. Management, 29, 172 (1965)
3. P. L. Ames, J. Appl. Ecol., 3 (suppl.), 87 (1966)
4. D. A. Ratcliffe, Bird Study, 14, 238 (1967)
5. J. J. Hickey, Peregrine Falcon Populations, Their Biology and Decline, University of Wisconsin Press, Madison, Wis. (1969)
6. C. F. Wurster and D. B. Wingate, Science, 159, #3818, 979 (1968)
7. S. Camp, Brit. Birds, 56, 124 (1963)
8. L. F. Stickel et al, The 31st Trans. of North American Wildlife Resources Conf., p. 190 (1966)
9. D. A. Ratcliffe and J. D. Lockie, Brit. Birds, 58, 65 (1965)
10. D. A. Ratcliffe, Nature (London), 215, 208 (1967)
11. J. J. Hickey and D. W. Anderson, Science, 162, 271 (1968)
12. N. W. Moore and J. Totton, Nature, 207, #4992, 42 (1965)
13. D. A. Ratcliffe, Bird Study, 12, 66 (1965)
14. I. Prestt, University of Wisconsin Publications (1967)
15. C. F. Wurster, Bioscience, August, 1969, 19, #9, 809(1969)
16. R. G. Heath, J. W. Spann and J. R. Kreitzer, Nature 224, #5214, 47 (1969)
17. Joel Bitman, H. C. Cecil, S. J. Harris, G. F. Fries, Nature, 224, #5214, 44 (1969)

18. D. A. Ratcliffe, Brit. Birds, 51, 23,(1958)

19. J. D. Jefferies, Ibid., 109, 266, (1967)

20. D. B. Peakall, Nature (London), 216, 505, (1967)

21. R. M. Welsh, W. Levin and A. H. Conney, J. of Pharmac. and Exper. Therapy, 155, #1, 167, (1967)

22. W. B. Deichmann, W. E. MacDonald, A. G. Beasley, D. Cubit, Subnormal Reproduction in Beagle Dogs Induced by D. D. T. and Aldrin, Ind. Med., 40, #2, 10, (1971)

23. John J. Meister, Candidacy Examination Report, Proposition #1, D.D.T. Effects on Androgenic Steroids in Man, California Institute of Technology, (1970)

24. M. L. E. Espir, J. W. Hall, J. G. Shirreffs, D. L. Stevens, Impotence in Farm Workers Using Toxic Chemicals, Brit. Med. J., 1, 423, (1970)

25. R. M. Welsch, W. Levin, A. H. Conney, Estrogenic Action of D. D. T. and its Analogs, Toxicol. Appl. Pharmacol., 14, 358, (1969)

26. Irma West, Pesticides as Contaminants, Arch. Environ. Health, 9, 626, (1964)

27. G. E. Quinby, John F. Armstrong, William F. Durham, D. D. T. in Human Milk, Nature 207, #4998, 726, (1965)

28. August Curley, Renate D. Kimbrough, Arch. Environ. Health, 18, 156, (1969)

29. W. E. J. Phillips, G. Hatina, D. C. Villeneuye, D. L. Grant, Multigeneration Studies of the Effects of Dietary

D. D. T. on the Vitamin A Status of the Weanling Rat, Can. J. Physiol. Pharmacol., 49, 382, (1971)

30. H. Burlington, V. F. Lindeman, Effect of D. D. T. on Testes and Secondary Sex Characteristics of White Leghorn Cockerels, Proc. Soc. Exp. Biol. Med. 74, 48, (1950)

ABSTRACT OF PROPOSITION THREE

Complex number calculations are currently conducted on a single complex plane with a branch cut. As a result, uniqueness and closure problems arise in arithmetic operations. A computer language COMPLEX is defined which removes the numerical difficulties of calculations on the complex plane by operating on the Riemann Spiral.

Proposition: A specially designed computer language, COMPLEX can remove the uniqueness and reversibility problems which currently plague calculations on the complex plane.

The set of complex numbers commonly used in studies of functions on the complex plane is not a closed and unique set. This set is actually one small subset of the full set of complex numbers obtained by applying the restriction,

$$C_0 = \{ z \mid z = re^{i\theta}, \ -\pi < \theta \leq \pi \}, \qquad (1)$$

to all complex numbers. The set C_0 is the standard $x + iy$ complex plane.

However, standard operations on the elements of C_0 yield results which are not elements of the set C_0 (Mc50). Consider as an example of this phenomena, the problem of raising i to the tenth power.

$$i^{10} = e^{10 \operatorname{Log} i} = e^{i 5 \pi}.$$

Even though 10 and i are elements of C_0, the result of raising i to the tenth power, $e^{i 5 \pi}$, is not an element of C_0. Using the definition

$$C_n \equiv \{ z \mid z = re^{i\theta}, \ (2n-1)\pi < \theta \leq (2n+1)\pi \}, \qquad (2)$$

To specify the infinite sequence of complex sets, C_n, allows $e^{i5\pi}$ to be fixed as a member of the set C_2.

The lack of a closure property in each set C_n is usually skirted by defining a branch cut on the complex plane (Ne61, Ne70). The branch cut is nothing more than a rule by which the results of

any operation on the elements of C_n are reduced to a representation in elements of C_n. The rule for the set C_0 would be that all calculations must be performed modulo 2π. Thus,

$$e^{i5\pi} \rightarrow e^{i\pi},$$

and i^{10} can be represented as an element of C_0. Unfortunately, branch cuts cause uniqueness problems on the complex plane because

$$(i^{10})^{1/10} \neq (e^{i\pi})^{1/10} = .9511 + .0390i .$$

In a numerical calculation, the imposition of a branch cut must be very carefully applied. As the above example shows, random application of a branch cut results in data which is incorrect by a phase value. Because a branch cut must be consistantly applied and this "consistancy" is based on the ultimate goal of the calculation as well as past calculations performed on the data, branch cuts cannot be readily imposed in computational treatment of a problem on the complex plane.

The Riemann Spiral:

The difficulties of manipulating complex values on a computer can be removed by performing all calculations on the Riemann Spiral (Ah53, Ah71). The Riemann Spiral is one representation of the set of all complex numbers. The concept of the Riemann Spiral was disclosed by Bernhard Riemann in his inaugural dissertation, Grundlagen fur eine allgemeine theorie der Functionen einer veranderlichen complexen Grosse, published on December 25, 1851. A diagram of the structure of the spiral

is shown in Figure 3.1. The spiral is the concatination of all elements of the infinite sequence of sets, C_n, into one set $\mathfrak{R}$.

The set $\mathfrak{R}$ is closed under addition and multiplication, is infinitely non-denumerable and is unique under its two set operations (Ha61). These properties are sufficient to resolve the ambiguities of computer calculations on the complex plane and they can be applied to this problem via the computer compiler COMPLEX.

The computer language COMPLEX will be a scientific, numerical calculation language designed to conduct its analyses on the Riemann Spiral. Basic to this language is the representation of all numbers as a three element array. All numbers manipulated by this language are treated as full complex numbers with no integer or real numbers maintained as a separate subset of numerical data.

Any number will be an ordered string of three elements. The sequence of parts in the number will be

$$(X, Y, n). \qquad (3)$$

The values X and Y are the components of the representation $z = x + iy$ while the third element, n, is the value of the subscript of the set of definition 2), C_n, to which $z = x + iy$ belongs. No number will be overtly represented in the syntax of the language as a three element array, Instead, for each numerical variable encountered in a source deck, the COMPLEX compiler will establish three ordered storage locations which will represent

that particular numerical data element for the duration of the calculation. These three storage elements will be manipulated as a unit in all, save a very few, calculations.

The compiler's addition and additive inverse operation are conducted on the number form of equation 3). The definition of the result is

$$z_1 + z_2 = (x_1, y_1, n_1) + (x_2, y_2, n_2) = (x_1 + x_2, y_1 + y_2, n_1 + n_2).$$

The additive idenity element will be (0, 0, 0).

The multiplication and multiplicative inverse operation will be conducted on number elements in their polar form. The definition of the result is

$$z_1 z_2 = r_1 e^{i(2n_1\pi + \theta_1)} \times r_2 e^{i(2n_2\pi + \theta_2)} = r_1 r_2 e^{i(2[n_1 + n_2]\pi + \theta_1 + \theta_2)}.$$

The multiplicative idenity element will be (1, 0, 0).

The syntax of the language COMPLEX will be based on the language FORTRAN IV (An66). A submitted source package must contain a main program while any specialized operations can be included in the source package as functions or subroutines. Any statement must be contained on one standard computer card with the statement beginning in or after column 7 and extending toward but not into column 73. Statements can be continued over several cards by a column 6 entry in the continuation cards.

Parsing of the source input will be done by bounded context analysis by precidence (Ch59, F163, F164). Declarations will be handled with a symbol table (F161, Ev64). The preci-

dence hierarchy for this language is

a) Evaluation of subroutines or functions.

b) Evaluation of unitary minius.

c) Exponentiation.

d) Divide.

e) Multiply.

f) Subtract.

g) Add.

h) Logical operations:

1. Less Than
2. Less Than or Equal To
3. Equal To
4. Not Equal To
5. Greater Than
6. Greater Than or Equal To
7. Not
8. And
9. Or

i) Equate variables.

Character recognition will be achieved by binary cut, digital comparison. The parentheses pair () act as delimiters on the precidence parsing with the parse proceeding from the innermost expression outward (Sa60). Elements of equal precidence in a given statement will be evaluated from left to right in order of appearance in the statement.

Two degrees of accuracy may be specified in any numerical calculation. These accuracy levels will be the single and double precision arithemetic modes of computition and they will provide m digit and 2m digit accuracy, respectively. Since all numbers manipulated by COMPLEX are three term, complex numbers, the single and double precision labels provide the only numerical variable types in this language. Real and integer variables may not exist.

All numbers, arrays and expressions will be processed to machine code by the compiler and organized and sequenced with Thunks (In61). A set of special functions titled, REAL, IMAG and SET access the X value, the Y value or the n value of any complex number treated by this language. All logical comparisons of magnitude such as "greater than" or "less than" will be done in real arithmatic. The one exception will be the comparison "equal to". Two numbers will be equal only if all three of their corresponding parts are equal.

The base used to represent all input material, the byte length of data, the exponent and sign convention and the size limit on data are all system dependent items. They will therefore vary from machine to machine. All numerical data read into the compiler must consist of ordered, three element strings. There will be no default options to compact a numerical data set save the

blank field = understood zero

rule already present in several languages (IB71, Wi66).

The three element rule will affect DATA and assignment statements. Each assigned number will be an ordered sequence of three numbers separated by commas, giving the assignment the form:

Variable = #.##, #.##, ## .

An error statement will be triggered by any input process which does not bring in a complete set of three numbers for each variable to be assigned.

The language COMPLEX will transfer all data between program sections by location (IB70). There will be no data transfers by form or value.

With this computer language, the uniqueness and branch cut problems formerly encountered in calculations in complex arithmatic are vanquished. The language COMPLEX allows numerical calculations in the complex field to be conducted in the same manner as any other computer calculation.

3: Figure Caption

Figure 3.1: The Riemann Spiral showing sets C_{-1}, C_0, C_1. The element (r, θ) is a member of the set C_0.

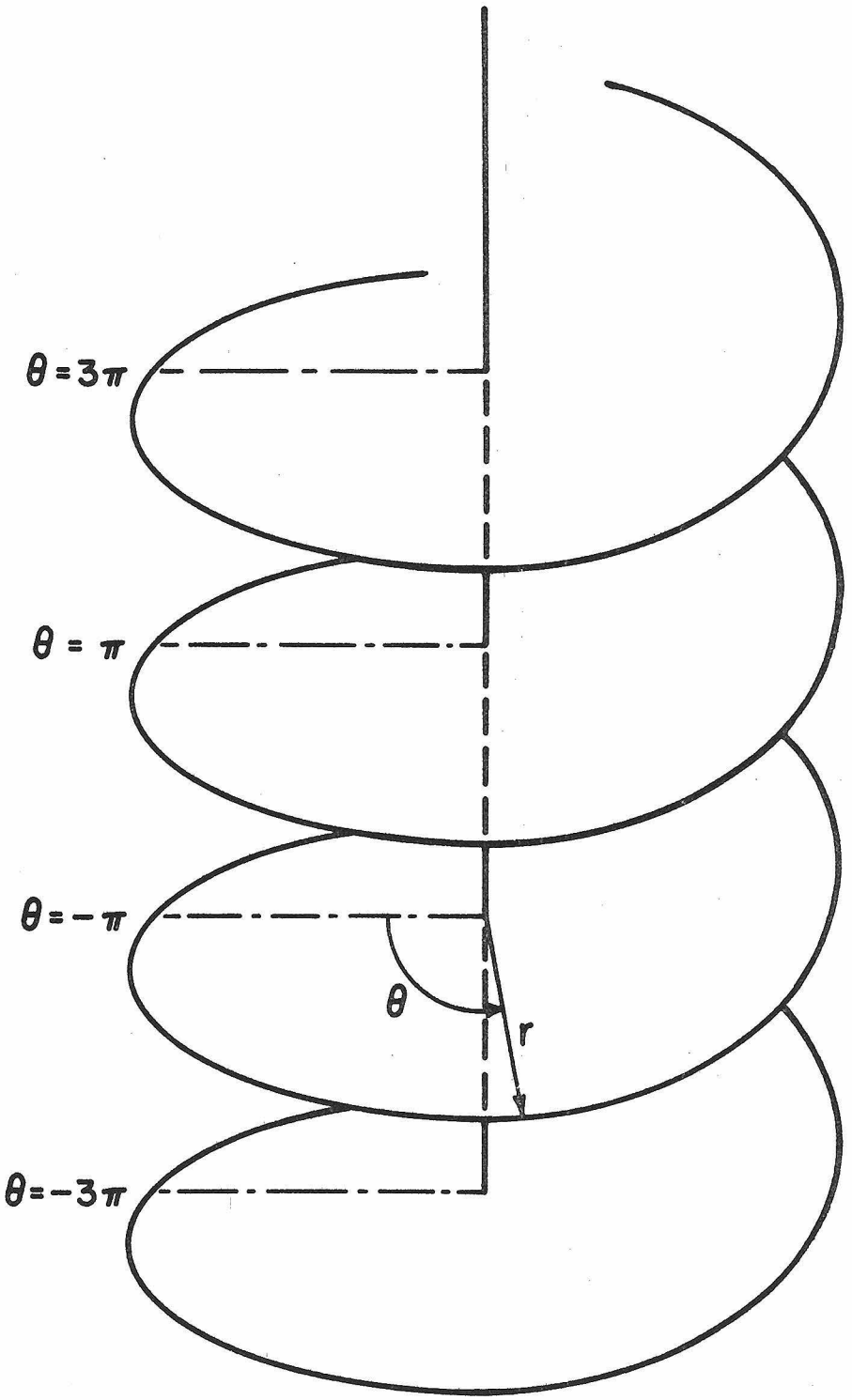


Figure 3.1

3. References

Ah53 L. Ahlfors, E. Calabi, M. Morse, L. Sario, D. Spercer, Contributions to the Theory of Reimann Surfaces, Annals of Mathematical Studies, Number 30, Princeton University Press, (1953)

Ah71 L. V. Ahlfors, L. Bers, Advances in the Theory of Riemann Surfaces, Proceedings of the 1969 Stony Brook Conference, Princeton University Press, (1971)

An66 Decima M. Anderson, Computer Programming FORTRAN IV, Appleton-Century-Crofts, (1966)

Ch59 N. Chamsky, On Certain Formal Properties of Grammers, Inform. Cont., 2, 137, (1959); 2, 393, (1959).

Ev64 A. Evans Jnr., An Algol 60 Compiler, Annual Review of Automatic Programming, 4, 87, (1964), Pergamon Press

Fl61 Robert W. Floyd, A Descriptive Language for Symbol Manipulation, Jour. Assoc. Comp. Mach., 8, 579, (1961)

Fl63 Rogert W. Floyd, Syntactic Analysis and Operator Precidence, Jour. Assoc. Comp. Mach., 10, #3, 316, (1963)

Fl64 Robert W. Floyd, Bounded Context Syntactic Analysis, Comm. Assoc. Comp. Mach., 7, #2, 62, (1964)

Ha61 Norman Hamilton, Joseph Landin, Set Theory and the Structure of Arithmetic, p. 253, Allyn and Bacon Inc., (1961)

IB70 IBM Systems Reference Library, Fortran IV (G and H) Programmer's Guide, p. 146, S360-25, GC28-6817-2,

International Business Machines Corp., (1970)

IB71 IBM System/360 and System/370 Fortran IV Language, GC28-6515-8, International Business Machines Corp., (1971)

In61 P. Z. Ingerman, Thunks, Comm. Assoc. Comp. Mach., 4, #1, 55, (1961)

Mc50 Thomas M. MacRobert, Functions of a Complex Variable, Chapter 2, Macmillan and Co., London, (1950)

Ne61 Zeev Nehari, Introduction to Complex Analysis, Chapter 2, p. 49, Allyn and Bacon Inc., (1961)

Ne70 Rolf Nevanlinna, Analytic Functions, p. 323, Springer-Verlag, New York, (1970)

Sa60 K. Samelson, F. L. Bauer, Sequential Formula Translation, Comm. Assoc. Comp. Mach., 3, 76, (1960)

Wi66 N. Wirth and H. Weber, EULER, A Generalization of ALGOL and its Formal Definition, Comm. Assoc. Comp. Mach., 9. 13, (1966); 9, 88, (1966)

ABSTRACT OF PROPOSITION FOUR

Several basic concepts have been used to explain the growth of suburban zones about the metropolitan centers of the United States. These explainations have generally ignored the economic forces generated by industrial decentralization and thus imply that the movement of population to the suburbs is promoted generally by class or racial forces or by repugnant characteristics of the urban region. As industry moves to the suburbs, the availability of suburban employment draws people from the urban core and therefore, industrial relocation acts as a significant cause of urban to suburban population movement.

Proposition: At some point in time during the development of a suburban residential ring about a typical core city, industrial decentralization and the availability of suburban jobs becomes a significant force in drawing population into the suburban region.

In recent years, there have been many fundamental changes in the structure of American society. To effectively discuss one particular structural characteristic, the current agglomeration pattern of a population in an urban region, a number of definitions must first be established.

The population centers treated in this discussion will be the 247 Standard Metropolitan Statistical Areas of the 1970 United States Census (US67, US72). The term urban area will generally be applied to that region within the jurisdictional boundaries of the city or cities comprising the core unit of the Standard Metropolitan Statistical Area (SMSA). The term suburb will be applied to all parts of the SMSA not contained in the core city or cities (US68).

Changes in a person's usual place of residence are generally broken into two types. The first type of change is the local move, a change of residence in the same community. The second type of move is migration, changes of community as well as residence. The current Bureau of the Census classification of mobility status and type of mobility (US63) is

Mobility Status		Type of Mobility
I.	Living in same house	Nonmover
II.	Living in different house in same county	Intracounty mover
III.	Living in different county	Migrant
	A. Same State	Intrastate migrant
	B. Different State	Interstate migrant
	1. Contiguous States	-
	2. Noncontiguous States	-

For the purposes of this study, each change of residence considered will be a local move within one SMSA from the urban core of this SMSA to its suburban area. Because of the extent of most Standard Metropolitan Statistical Areas, these local moves will represent all classes of the Bureau of the Census mobility status listing.

Past Mobility Models

From 1930 onward, the suburban ring of most United States SMSA's gained a larger fraction of the total population growth of the entire area than did the core city. Table 4.1 shows the rapid population increase in the suburban region of U.S. metropolitan areas by both race and census year. The Population listing shows the rapid increase in numbers of people outside the central city. The Percent of Change listing of Table 4.1 shows the differential rate of increase of urban versus suburban population while the Percent by Race and Percent by Residence

and Race Tabulations show that this has been an overwhelmingly caucasian movement. Bogue et al established in 1953 that this developing residency pattern was the result of shifts in population from the urban cores of the SMSA's to their suburban rings (Bo53, Bo57).

Since the vanguard studies of Goodrich and Thorthwaite (Go36, Th34) on population migration, a number of social models explaining regional movement have been put forward.

A number of these explainatory descriptions of population movements have applied directly to the area of urban to suburban population flow.

The major concepts of each of four ideologies which have been used to explain urban to suburban moves will be discussed. These four ideologies are

A) White Flight movement

B) Change of Life moves

C) Rural to Metropolitan migration

D) The Urban Draw, Suburban Flow Process.

The White Flight image of why suburbs grow is based on the idea that the caucasian fraction of the population, moves to the suburban ring of the metropolitan area to escape the taxes, the conjestion and the minority groups which are all increasing in the city. The pattern of racial segregation implicit in Table 4.1 is projected to 1985 in Table 4.2. Because of the rapid separation of the races that these data portend, the concept that

the caucasian groups are vacating the urban regions was given gross statistical credance. In actuality, as Table 4.3 displays, the process of suburban movement was not so much an effort at racial separation as it was a process of economic separation.

The Change of Life picture of urban-suburban residence change is based on the belief that at certain transition points in every individual's life, his or her probability of changing abode is high. This causual concept of mobility has been investigated for several movement initiating transitions. Reaching the age of legal adulthood is a well established transition point for initiating migration (Sh65). Marriage is a second force which promotes a change of residence (US71). One final period specific change which often causes a move is the birth of an additional child (Ne70). Life cycle influences upon mobility are extensively analysed in Sp70.

The Rural to Metropolitan migration of the U.S. population has become a very small part of the total migration flows that compose our population movement. The reason that rural to metropolitan migration has become an insignificant feature of total population mobility is simply that the U.S. rural population has become so small that it lacks sufficient numbers to influence migration rates. A discussion of rural-metropolitan migration patterns will be found in US65. The forces which have replaced rural to metropolitan migration as a source of metropolitan growth are natural increase, intermetropolitan migration and

immigration (Co72).

A recent phenomena in metropolitan growth has been the Urban Draw, Suburban Flow Process (Mo72b). In this sequence of moves, the population tends to flow from one urban area to another in the first phase of the migration process. Soon thereafter, however, the same group of movers change their residence to an area in the suburbs of the SMSA. There are some indications at the present time that the standard rural to metropolitan migration of the past two centuries has been absorbed into this two step settlement process.

The current models for population relocation definately explain a significant portion of the urban to suburban population flow that is occuring in the United States. Yet there do appear to be other forces that are drawing people out of the core cities of most SMSA's. One such force of fairly recent vintage is, I suspect, the economic drawing power of suburban industry.

Economic motivation for a change of residence is well established as an initiator of migration (Go36). While the original concept that Labor flows from economically depressed areas to economically prosperous areas has been shown to be too simplistic to describe most migration processes (La67, Mo72), jobs and increased employment potential are well established motivators of migration (Sa64). Coupling this datum with comparisions of the 1963 and 1967 Census of Manufacturers (US66, US71b) suggests that suburban growth is now continuing because personnel

are being recruited from urban cores for jobs in suburban industries. The two Censuses of Manufacturers and other independent data (Ne67), show that industry is moving out of the city. As major industries move into the suburban ring and service industries arise to cater to the needs of the suburban population, job opportunities appear in the suburban region of each Standard Metropolitan Statistical Area. These job openings will be filled by both suburban residents and residents of the urban core.

Once the economic force of available jobs has arisen in the suburban area, a movement of place of residence from the urban core to the suburban ring will occur as the mobile group locates near its place of employment. While proximity to employment is normally not a major criteria which is weighed in making a move (Bu69), the additional attractive features of the suburban location will weigh heavily in favor of a change of residence.

To date, no study has been made of the significance of the suburban movement of population initiated by the decentralization of industry. Such a study can be conducted in several stages to clarify what fraction of suburban movement is due to the economic opportunities of the suburb.

The first stage of this study can be conducted on data for industrial decentralization from the Department of Labor and on data for urban to suburban residential change from the Bureau of the Census. The general feature of identical flow directions has already been established (Ne67, Ho68). A time correlation on

this data will provide the final feature needed to complete this stage of the study.

The second phase of this investigation will be an analysis of the address changes of the workers of a statistically representative group of recently established suburban industries. This test of the suburban, economic draw idea should disclose that a significant fraction of urban to suburban relocations occurred after suburban employment was obtained.

If the expected results are found in the first two sections of this inquiry, then a final motivation check will be made on a representative sample of workers in the relocated industries. This inquiry into the duration of the individual's current place of residence and the motivation for any changes of residence will completely define the contribution industrial development in the suburbs is making to urban core depopulation. This final study will be done either by mailed questionnaire or personal interview.

Several issues of social policy that are presently receiving wide attention mandate that the forces promoting population movement to the suburbs be fully understood. A classic example of these issues is the current debate over land use policies. The question of whether statewide zoning and regional development control will be benificial or inhibitory should not be resolved in a state of ignorance of the basic migratory process.

Similarly, the recommendations of the National Commission on Urban Problems (Co69a) and the proposals of the National

Commission on the Causes and Prevention of Violence (Co69b) would be affected significantly if suburban industrial draw is shown to be a major cause of residency change. Under Fair Employment Practices hiring, the racial communities of the United States will be desegregated by the steady movement of urban minority labor to suburban employment.

Table 4.1 Population Inside And Outside Central City Or Cities Of Standard Metropolitan Statistical Areas, By Race: 1900 To 1960.

United States And Regions

(Numbers in Thousands. Percent not shown where less than 0.1 or where base is less than 100. Source US63b.)

Area And Subject	All Classes			White			Negro		
	Total	Central City	Outside Central City	Total	Central City	Outside Central City	Total	Central City	Outside Central City
United States									
Population									
1960.....	112 885	58 004	54 881	99 688	47 655	52 033	12 198	9 705	2 493
1950.....	89 317	42 386	36 931	80 343	45 499	34 844	8 360	6 456	1 904
1940.....	72 834	45 652	27 182	66 570	41 021	25 548	5 840	4 358	1 482
1930.....	66 915	43 207	23 708	61 528	39 337	22 191	4 991	3 634	1 357
1920.....	52 631	34 725	17 907	48 836	32 192	16 644	3 547	2 382	1 165
1910.....	42 094	27 175	14 919	39 007	25 302	13 704	2 820	1 703	1 117
1900.....	31 895	19 825	12 070	29 413	18 480	10 934	2 352	1 281	1 071

Table 4.1 (continued)

Area And Subject	All Classes			White			Negro		
	Total	Central City	Outside Central City	Total	Central City	Outside Central City	Total	Central City	Outside Central City
Amount of Change									
1950 to 1960.....	23 568	5 619	17 950	19 344	2 155	17 189	3 939	3 249	589
1940 to 1950.....	16 482	6 733	9 749	13 774	4 478	9 296	2 620	2 098	422
1930 to 1940.....	5 919	2 445	3 474	5 042	1 685	3 357	849	724	125
1920 to 1930.....	14 284	8 483	5 801	12 691	7 145	5 547	1 444	1 251	192
1910 to 1920.....	10 537	7 550	2 987	9 830	6 890	2 940	728	680	48
1900 to 1910.....	10 199	7 350	2 840	9 593	6 823	2 771	468	422	46
Percent of Change									
1950 to 1960.....	26.4	10.7	48.6	24.1	4.7	49.3	45.9	50.3	30.9
1940 to 1950.....	22.6	14.7	36.9	20.7	10.9	36.5	43.2	48.1	28.5
1930 to 1940.....	8.8	5.7	14.7	8.2	4.3	15.1	17.0	19.9	9.2
1920 to 1930.....	27.1	24.4	32.4	26.0	22.2	33.3	40.7	62.5	15.5
1910 to 1920.....	25.0	27.8	20.0	25.2	27.2	21.5	25.8	29.9	4.3
1900 to 1910.....	32.0	37.1	23.6	32.6	36.9	25.3	19.9	32.9	4.3

Table 4.1 (continued)

Area And Subject	All Classes			White			Negro		
	Total	Central City	Outside Central City	Total	Central City	Outside Central City	Total	Central City	Outside Central City
Percent By Residence And Race									
1960.....	100.0	51.4	48.6	88.3	42.2	46.1	10.8	8.6	2.2
1950.....	100.0	58.7	41.3	90.0	50.9	39.0	9.4	7.2	2.1
1940.....	100.0	62.7	37.3	91.4	56.3	35.1	8.0	6.0	2.0
1930.....	100.0	64.6	35.4	91.9	58.8	33.2	7.5	5.4	2.0
1920.....	100.0	66.0	34.0	92.8	61.2	31.6	6.7	4.5	2.2
1910.....	100.0	64.6	35.4	92.7	60.1	32.6	6.7	4.0	2.7
1900.....	100.0	62.2	37.8	92.2	57.9	34.3	7.4	4.0	3.4

Table 4.2 Projected Growth 1960 to 1985 Within Component Parts of Metropolitan* Areas by Color and by Region.

[Numbers in Thousands. Source Ho68.]

Region, Color and Residence.	1985	1960	Increase 1960 to 1985 Number	Increase 1960 to 1985 Percent	Percent by Residence within SMSA's 1985	Percent by Residence within SMSA's 1960	Change
United States							
White	151 164	99 692	51 472	51.6	100.0	100.0	-
Central City	45 435	47 852	-2 417	-5.0	30.1	48.0	-17.9
Ring	105 730	51 840	53 890	104.0	69.9	52.0	17.9
Nonwhite	26 974	13 192	13 782	104.6	100.0	100.0	-
Central City	20 146	10 356	9 790	94.5	74.7	78.5	-3.8
Ring	6 827	2 836	3 991	140.7	25.3	21.5	3.8
Northeast							
White	41 423	32 388	9 035	27.9	100.0	100.0	-
Central City	13 485	14 925	-1 440	-9.6	32.6	46.1	-13.5
Ring	27 938	17 463	10 475	60.0	67.4	53.9	13.5
Nonwhite	5 905	2 962	2 943	99.4	100.0	100.0	-
Central City	4 833	2 398	2 435	101.5	81.8	81.0	0.8
Ring	1 072	564	508	90.1	18.2	19.0	-0.8

* 1960 boundaries of SMSA's used for 1960; 1967 boundaries used for 1985 calculations.

Table 4.2 (continued)

Region, Color and Residence.	1985	1960	Increase 1960 to 1985 Number	Increase 1960 to 1985 Percent	Percent by Residence within SMSA's 1985	Percent by Residence within SMSA's 1960	Change
North Central							
White	38 698	27 718	10 980	39.6	100.0	100.0	-
Central City	11 326	13 793	-2 467	-17.9	29.3	49.8	-20.5
Ring	27 372	13 925	13 447	96.9	70.7	50.2	20.5
Nonwhite	5 944	3 245	2 699	83.2	100.0	100.0	-
Central City	5 318	2 849	2 469	86.7	89.5	87.8	1.7
Ring	627	396	231	58.3	10.5	12.2	-1.7
South							
White	35 362	21 183	14 179	66.9	100.0	100.0	-
Central City	11 236	11 144	92	0.8	31.8	52.6	-20.8
Ring	24 126	10 039	14 087	140.3	68.2	47.4	20.8
Nonwhite	10 794	5 253	5 541	105.5	100.0	100.0	-
Central City	7 137	3 918	3 219	82.2	66.1	74.6	-8.5
Ring	3 658	1 335	2 323	174.0	33.9	25.4	8.5

Table 4.2 (continued)

Region, Color and Residence.	1985	1960	Increase 1960 to 1985 Number	Increase 1960 to 1985 Percent	Percent by Residence within SMSA's 1985	Percent by Residence within SMSA's 1960	Change
West							
White	35 682	18 403	17 279	93.9	100.0	100.0	-
Central City	9 388	7 990	1 398	17.5	26.3	43.4	-17.1
Ring	25 294	10 413	15 881	152.5	73.7	56.6	17.1
Nonwhite	4 330	1 732	2 598	150.0	100.0	100.0	-
Central City	2 959	1 190	1 669	140.3	66.0	68.7	-2.7
Ring	1 470	542	928	171.2	34.0	31.3	2.7

Table 4.3 Income In 1959 Of Families By Color Of Head Of Family For Standard Metropolitan Statistical Areas, Central Cities, And Outside Central Cities: 1960.

United States And Regions

(Numbers in Thousands. Percent not shown where less than 0.1 or where base is less than 400. Source US63c)

Area And Subject	All Classes			White			Negro		
	Total	Central City	Outside Central City	Total	Central City	Outside Central City	Total	Central City	Outside Central City
United States									
Families With Income									
Total.....	28 620	14 743	13 877	25 773	12 457	12 316	2 847	2 287	561
Under $3,000.....	4 336	2 596	1 740	3 308	1 790	1 519	1 028	807	221
$3,000 to $9,999...	18 899	9 709	9 190	17 241	8 358	8 883	1 658	1 350	307
$10,000 And Over..	5 385	2 438	2 947	5 223	2 309	2 915	162	129	32
Under $3,000 or $10,000 And Over..	9 721	5 034	4 687	8 532	4 098	4 433	1 190	936	253
Percent By Income .	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0
Under $3,000.....	15.1	17.6	12.5	12.8	14.4	11.4	36.1	35.3	39.4
$3,000 to $9,999...	66.0	65.9	66.2	66.9	67.1	66.7	58.2	59.1	54.8
$10,000 And Over .	18.8	16.5	21.2	20.3	18.5	21.9	5.7	5.7	5.8

Table 4.3 (continued)

Area And Subject	All Classes			White			Negro		
	Total	Central City	Outside Central City	Total	Central City	Outside Central City	Total	Central City	Outside Central City
Percent By Residence.....	100.0	52.5	48.6	100.0	48.3	51.7	100.0	80.3	19.7
Under $3,000.....	100.0	59.9	40.1	100.0	54.1	45.9	100.0	78.5	21.5
$3,000 to $9,999...	100.0	51.4	48.6	100.0	48.5	51.5	100.0	81.5	18.5
$10,000 And Over..	100.0	45.3	54.7	100.0	44.2	55.8	100.0	79.9	20.1
Percent By Color...	100.0	100.0	100.0	90.1	84.5	96.0	9.9	15.5	4.0
Under $3,000.....	100.0	100.0	100.0	76.3	68.9	87.3	23.7	31.1	12.7
$3,000 to $9,999...	100.0	100.0	100.0	91.2	86.1	96.7	8.8	13.9	2.2
$10,000 And Over..	100.0	100.0	100.0	97.0	94.7	98.9	3.0	5.3	1.1
Percent By Residence And Color.....	100.0	51.5	48.5	90.1	43.5	46.5	9.9	8.0	2.0
Under $3,000.....	100.0	59.9	40.1	76.3	41.3	35.0	23.7	18.6	6.1
$3,000 to $9,999...	100.0	51.4	48.6	91.2	44.2	47.0	9.9	7.1	1.6
$10,000 And Over..	100.0	45.3	54.7	97.0	42.9	54.1	3.0	2.4	0.6

Table 4.3 (continued)

Area And Subject	All Classes			White			Negro		
	Total	Central City	Outside Central City	Total	Central City	Outside Central City	Total	Central City	Outside Central City
Ratios									
Number Outside Central City Per 100 In Central City									
Families With Income	...	100.0	94.1	...	100.0	106.9	...	100.0	24.5
Under $3,000.....	...	100.0	67.0	...	100.0	84.9	...	100.0	27.4
$3,000 to $9,999 ..	...	100.0	94.7	...	100.0	106.3	...	100.0	22.8
$10,000 And Over..	...	100.0	120.9	...	100.0	126.3	...	100.0	25.1
Nonwhites Per 100 Whites									
Families With Income	...	...	...	100.0	100.0	100.0	11.0	18.4	4.2
Under $3,000.....	...	...	...	100.0	100.0	100.0	31.1	45.1	14.5
$3,000 to $9,999 ...	...	...	...	100.0	100.0	100.0	9.6	16.2	3.5
$10,000 And Over...	...	...	...	100.0	100.0	100.0	3.1	6.6	1.1

4: References

Be68 Brian J. L. Berry, Peter G. Goheen, Harold Goldstein, Metropolitan Area Definition: A Re-Evaluation of Concept and Statistical Practice, Burear of the Census, U.S. Department of Commerce, Working Paper #28,(1968)

Bo53 Donald J. Bogue, Henry S. Shryock, Jr., Siegfried A. Hoermann, Subregional Migration in the United States, 1935-40. Volume 1: Streams of Migration Between Subregions, Scripps Foundation for Research in Population Problems, (1953)

Bo57 Donald J. Bogue, Margaret J. Hargood, Gladys K. Bowles, Subregional Migration in the United States, 1935-40, Volume 2, Differential Migration in the Corn and Cotton Belts, Scripps Foundation for Research in Population Problems, (1957)

Bu69 Edgar Butler, Moving Behavior and Residential Choice: A National Survey, National Cooperative Highway Research Program, National Academy of Sciences, (1969)

Co69a National Commission on Urban Problems, Building the American City, Frederick A. Praeger Publishers, (1969)

Co69b National Commission on the Causes and Prevention of Violence, To Establish Justice, To Insure Domestic Tranquility, U.S. Government Printing Office, Washington, D.C., (1969)

Co72 The Commission on Population Growth and the American

Future, Population and the American Future, page 29, U.S. Government Printing Office, Washington, D.C., (1972)

Go36 Carter Goodrich and Associates, Migration and Economic Opportunity, University of Pennsylvania Press, (1936)

Ho68 Patricia Leavey Hodge, Philip M. Hauser, The Challange of America's Metropolitan Population Outlook, 1960 to 1985, page 26, Table III-5, Frederick A. Praeger, (1968)

La67 John B. Lansing, Eva Mueller, The Geographic Mobility of Labor, Survey Research Center, Institute for Social Research, (1967)

Mo72a Peter A. Morrison, Population Movements and the Shape of Urban Growth: Implications for Public Policy, Rand Corp. R-1072-CPG, August, (1972)

Mo72b Peter A. Morrison, Rand Corporation, Santa Monica, Private Communication, (1972)

Ne67 Dorothy K. Newman, The Decentralization of Jobs, Monthly Labor Review, 90, #5, 7, (1967)

Ne70 Jeanne S. Newman, Residential Mobility and the Timing of Marriage and Childbirth, Unpublished Paper, April, (1970)

Sa64 Samuel Saben, Geographic Mobility and Employment Status, March 1962- March 1963, Monthly Labor Review, 87, 876, (1964)

Sh65 Henry S. Shryock, Elizabeth A. Larmon, Some Longitudinal Data on Internal Migration, Demography, 2, 579, (1965)

Sp70 Alden Speare Jr., Home Ownership, Life Cycle Stage, and

Residential Mobility, Demography, 7, 449, (1970)

Th34 C. Warren Thornthwaite, Internal Migration in the United States, University of Pennsylvania Press, (1934)

US63a U.S. Bureau of the Census, U.S. Census of the Population: 1960. Subject Reports. Mobility for States and State Economic Areas, Final Report PC(2)-2B, U. S. Government Printing Office, Washington D.C., (1963)

US63b U.S. Bureau of the Census, U.S. Census of the Population: 1960. Selected Area Reports. Standard Metropolitan Statistical Areas. Final Report PC(3)-1D., Table 1, page 2 U.S. Government Printing Office, Washington, D.C., (1963)

US63c U.S. Bureau of the Census, U.S. Census of the Population: 1960. Selected Area Reports. Standard Metropolitan Statistical Areas. Final Report PC(3)-1D, Table 8, page 679, U.S. Government Printing Office, Washington, D.C., (1963)

US65 U.S. Bureau of the Census, Historical Statistics of the United States, Colonial Times to 1957; Continuation to 1962 and Revisions, U.S. Government Printing Office, Washington, D.C., (1965)

US66 U.S. Bureau of the Census, Census of Manufacturers 1963, Volume III, Area Statistics, U.S. Government Printing Office, Washington, D.C., (1966)

US67 Standard Metropolitan Statistical Areas: 1967, Bureau of the Budget, U.S. Government Printing Office, Washington,

D.C., (1967)

US71a U.S. Bureau of the Census, Current Population Reports, Table 5, page 14, Series P-20, No. 210, January 15, 1971

US71b U.S. Bureau of the Census, Census of Manufacturers 1967, Volume III, Area Statistics, Parts 1 and 2, U.S. Government Printing Office, Washington, D.C., (1971)

US72 Metropolitan Housing Characteristics, Final Report HC(2)-1, United States and Regions, Bureau of the Census, U.S. Department of Commerce, Appendix A, page Appendix-1, (1972)

ABSTRACT OF PROPOSITION FIVE

The two non-linear, multiloop feedback systems constructed by J. W. Forrester to model social structures are critically examined for their modeling capacity. The lack of a spacial structure, insufficient proof of causality in the models' analytic structure, a complete lack of calibration and an exceedingly simplistic form for the models, all mandate that the two systems are inadequate to represent the structures they are supposed to describe. These models will more accurately describe the behavior of the represented social structures if a spacial distribution is built into the models and both are calibrated to the structures they are designed to mimic.

Proposition: The Forrester social models contained in Urban Dynamics and World Dynamics have serious deficiences in structure. These deficiences can be partially alleviated by installing a spacial dimension in the models and calibrating them to the modeled structures.

A fundamental advance occurred in the study of many complicated orginizational structures in 1948 when Norbert Wiener (Wi48) authored an elucidation of the principles of feedback systems and thereby founded the dicipline of Cybernetics. Since many complicated systems involve man himself, the systems analysis approach to many areas of human endevor was adopted rapidly.

The earliest applications of systems modeling to the organizational structure of society were in the area of traffic analysis. Static models of regional traffic flow (Mi54, Ze62) greatly enhanced the predictive capacity of Highway Planning Departments and resulted in far better engineering in the resulting highway systems.

The same forces which drove highway engineers to model their traffic arteries prompted Regional Planning Commissions to model more complete social systems. Several static city models were created in the early 1960's in an effort to predict the commercial and residential patterns that arose in an urban area under specific policy decisions. These initial models, of which the CATS model (Ha61, Ch60), the POLIMETRIC model (Bo62, Se66, De64) and the Pittsburg model (Lo64) are exemplary, were

static, socio-economic urban models which attempted to predict the aggregate behavior of urban populations. The static nature of these models made it very difficult to model time dependent social phenomena however, and therefore, dynamic social models were developed in the period from 1965 to 1970.

There are three major dynamic, regional models of an urban system. These models are Crecine's Time-Oriented Metropolitan Model (Cr68), Batty's Spacial Dynamic Model (Ba71) and Forrester's Urban Dynamic model (Fo69). The modeling of social and interpersonal processes has been applied to areas other than urban structure. Examples of systems analysis in other areas are the administration studies by J. T. Dorsey (Do58), the studies of international relationships by M. A. Kaplan (Ka57), the crime rate analysis of R. L. Kyllonen (Ky67) and the racial distribution studies of S. L. Levine (Le68). Since I wish to analyse Forrester's models of social structure, I have concentrated on the most comparable social models published, namely the urban and regional models just mentioned. To facilitate an analysis of the two Forrester models, their gross features will be presented.

Two Social Models

Two social system models which were used to represent 1) an urban area and 2) the world, were published by Jay W. Forrester in 1969 and 1971 (Fo69, Fo71), respectively. These two models were termed preliminary by Forrester and were published because, in Forrester's words, "Only with wider com-

ment and criticism can the methods, the assumptions and the results be adequately evaluated." This discussion is intended to be an overall critique of the Forrester social modeling method, continuing, in a hopefully more rational way (Sh71, Le72), the analysis of the capacities of Forrester's social models and the place of these models amongst other simliar constructs.

The two social models exhibited by Forrester are both multi-loop, non-linear feedback systems, though the two system models described are fairly simple systems. The urban model is an open system with one major feedback loop with its environment. The world system is a closed system.

Description of the Urban Model

The urban model is a dynamic system with nine level elements and twenty two rate elements. The level elements are composed of three groups:

a) Business

b) Housing

c) Population,

each of which is broken into three subgroups. The list of level elements is

a1) New Enterprise

a2) Mature Business

a3) Declining Industry

b1) Premium Housing

b2) Worker Housing

b3) Underemployed Housing

c1) Managerial-Professional Personnel

c2) Labor Personnel

c3) Underemployed Personnel.

The twenty two controlling rate elements are

1) Underemployed Personnel Birth Rate

2) Underemployed Personnel Arrival Rate

3) Underemployed Personnel Departure Rate

4) Transition Rate from Underemployed to Labor Level

5) Transition Rate from Labor to Underemployed Level

6) Labor Personnel Birth Rate

7) Labor Personnel Arrival Rate

8) Labor Personnel Departure Rate

9) Transition Rate from Labor to Management-Professional Level

10) Management-Professional Birth Rate

11) Management-Professional Arrival Rate

12) Management-Professional Departure Rate

13) Premium Housing Construction Rate

14) Premium Housing Obsolescence Rate

15) Worker Housing Construction Rate

16) Worker Housing Obsolescence Rate

17) Low Cost Housing Program Construction Rate

18) Slum Housing Demolition Rate

19) New Enterprise Decline Rate

20) New Enterprise Construction Rate

21) Mature Business Decline Rate

22) Declining Industry Demolition Rate.

Connecting these two types of system elements are a series of information channels which constitute the control and response

portion of the feedback system. The three classes of information channels in a feedback system are:

1) Equilibrium Processes: These processes keep the system static. An equilibrium process constitutes a negative feedback loop.
2) Hemostatic Processes: These processes try to maintain equilibrium in the face of disturbances from the environment or other feedback loops. A hemostatic process constitutes a negative feedback loop.
2) Morphogenetic processes: These processes regulate against certain kinds of disturbance but increase organization in the system by responding to disturbances in the environment. A morphogenetic process constitutes a positive feedback loop.

The urban model contains examples of all three classes of information channels. The complete structure of the information channels for the urban model is discussed in Appendix A of Fo69.

The Business and Housing level elements of the urban model have their respective subgroups connected by time dependent unidirectional flows. The Population group of level elements has its subgroup connected by time dependent and social dependent flows.

Description of the World Model

The complete system structure of Forrester's world model is shown in Figure 5.1. There are 5 level elements, 7 rate

elements and 48 information channel elements in this simplified model. The 5 level elements are

a) Population
b) Capital Investment
c) Natural Resources
d) Pollution
e) Fraction of Capital Devoted To Agriculture,

while the 7 rate elements are

1) Birth Rate
2) Death Rate
3) Pollution Generation Rate
4) Pollution Absorption Rate
5) Natural Resource Usage Rate
6) Capital Investment Generation Rate
7) Capital Investment Discard Rate.

The 48 information channels can be decerned in Figure 5.1.

Forrester has performed a number of long term projection calculations with the two models he created. The primary thrust of his computations has been policy analysis but, as the following critique will show, the form of the social models makes any conclusions obtained from their use of very, very doubtful validity.

Analysis

The system characteristics of the two dynamic models just described will be reviewed under the six system dimensions established by Britton Harris (Ha67). These structural dimensions are

1) Descriptive versus Analytic
2) Holistic versus Partial

3) Macro versus Micro

4) Static versus Dynamic

5) Deterministic versus Probabilistic

6) Sumultanious versus Sequential.

Descriptive versus Analytic

A descriptive model is one which repeats the history of the actual structure for a specific period of time. An analytic model performs the activities of the modeled structure at any point in time and, in its extream case, for any environmental conditions the structure could encounter.

Forrester's models are both analytic. They are proportedly designed to give a first approximation to the actions of an urban area or the world under certain conditions. An analytic model is only useful if all of the causual relationships and dynamic relationships of the modeled structure are clearly understood. This is obviously not the case in large, aggregate, social structures. Hence, Forrester's models far outstrip the current knowledge of urban or regional interactions and thus, are constructed on very unstable foundations.

The causual organization of a model can be partially verified by 'calibrating' the model to the known behavior of the modeled structure. Forrester does note that he has attempted to calibrate part of his urban model to his mental image of how a city behaves. In chapter 2, page 14 of Fo69, he states:

"When first modeling a social system it is usually best to

model the general class of system rather than a specific system. Here, this means a model to represent the central processes common to all urban areas rather than to represent those of a specific area. The general model will be simpler and more basic because it omits the peripheral considerations that may be special to a particular place. It focuses on those system components that are always to be found interacting in urban growth and stagnation. The model should include only those processes necessary to the creation and correction of urban decay."

In chapter 3, page 38 of Fo69, Forrester states:

"The stages of an urban life cycle within a period of 250 years occur starting with empty land, growing to full land occupancy, maturing through a rapid realignment of internal urban balance, and emerging into an equilibrium characterized by stagnation with its unemployment, faltering industry, and increased taxes."

Forrester has thus calibrated his metropolitan model to a personal conviction of how an arbitary, representative metropolis should behave. The fact that his urban model then decays over a prolonged period constitutes merely a self-fulfilling prophasy. Above and beyond the lack of a specific metropolitan area to which he could calibrate the descriptive phase of his model, Forrester also makes gross and simplistic assumptions about the causual structure of both of his models. He makes a similar

sequence of arbitary assumptions to select his "central processes common to all". I have found no agreement in the literature beyond a majority concensus on the significance of economics and population, on the topic of what constitutes central urban or regional elements. The question of how significant social elements knit themselves together to form a process is completely unanswerable at the present time.

Additionally, it should be noted that the calibration process is usually conducted by extensive regression analysis on the parameters of the system model (Ba71). Forrester chooses his parameters arbitarily.

Because of their simplicity, their arbitary causality and variable selection and the lack of distinct calibration, Forrester's models fail completely as the analitical models they portend to be.

Holistic versus Partial

A holistic model is one which considers not only the total environment but the totality of ultimate effects, both direct and indirect, of given policies. A partial model concentrates on one particular subsystem of the total system and measures its changes while the remainder of the system is static.

Forrester poses his systems as holistic as seen by the fact that only one environmental feedback channel exists in the two models. This posture, in view of the very low degree of resolution in the models and the simplistic structure of the systems is extreamly inappropriate.

Before examining the completeness of the models, I will mention the boundary problems of Forrester's urban model. Stafford Beer's (Be59) injunction to experimenters concerning the scale of a system is, "The system we choose to define is a system because it contains interrelated parts, and is in some sence a complete whole in itself." For Forrester's urban model to be a complete holistic system, it must be self-determining, which, he argues (See pages 17 and 18, Fo69.), it is. However, both current city behavior and other specialists (Fr65) imply that metropolitan behavior is strongly controlled by regional and national policy.

Any holistic model must represent several areas of human endeavor. These areas have been termed environments and I will analyse the other aspects of Forrester's holistic models under the environment catagories defined by McLoughlin and Webster (Mc70). These catagories are:

a) The Political Environment

b) The Economic Environment

c) The Technological Environment

d) The Attitude Environment.

The Political Environment

The major action of the political environment is to convert the system into an adaptive system. Neither of Forrester's systems has any major components to act as a policy making body. Hence, the models carry forward the same policies and this,

coupled with their analytical dynamic nature, causes the models to diverge.

The Economic Environment

The degree of resolution of the economic aspects of Forrester's models is exceedingly poor. Those economic variables that are included in the models are very simplistically related. Major economic motivators such as wages, spending patterns and savings are not treated at all by these systems. Further, Forrester never distinguishes between basic variables which are independent of economic or social control and gravity variables which are drawn to various areas or levels by the basic variable changes. An example of this process would be the capacity of a major industry, a steel mill, to draw secondary commercial investment, restaurants and filling stations, to its periphery.

The Technological Environment

Technology has a pronounced effect on the structure of societies. However, the major medium through which technology acts, the spacial dimension, is missing from both of Forrester's models. Societies cover a specific land area and a good model must represent this spacial distribution. Further, there are strong indications that the social and spacial structures of cities are both involved in hemostatic processes (Be62) and, as Batty (Ba71) notes, up to half of all changes in a system are changes in location rather than changes in levels of the system.

Technology should also have a noticeable impact on com-

munications, resource flows and productivity. These levels are almost completely ignored by the models, however.

The Attitude Environment

The significance of social attitudes in maintaining order in a society is a topic of extensive debate in the social sciences. At present, most individuals have avoided any explicit value variables in the models currently in operation. All models are governed by an implicit set of values and have a value structure which has controlled the models' development. As has already been noted, Forrester's urban model has an urban decay value system as an implicit component of its structure.

Macro versus Micro

A macroscopic model deals with variables which measure a total of a particular element. Microscopic models deal with each individual contribution to a system element.

Forrester's models are decisively macroscopic. This has generally been the case in all models that have been built. However, the degree of resolution of Forrester's work is so low that he must, if his social systems are to be taken seriously, treat his system components far more microscopically.

Static versus Dynamic

A static model either develops results for one particular time or projects its input data to some future time by a system of fixed formulas. A dynamic model propagates its input data forward in time, allowing the data to adjust the model's behavior

sequentially as the system advances to a final time status.

Forrester's models are complete analytical, dynamic models. While this class of models is undoubtably the most appropriate means of representing social structures, the models of this class are very unstable. Analytic, dynamic models require closure in the system and thus, tend to center all controls within the model. Hence, if one level or flow of the system becomes unbalanced, any model which is not strongly self-equilibrating will degenerate. Forrester's world model behaves in precisely this manner.

Something that is missing from these systems is a set of gravity models for some of the subsystems of the total construct. Gravity models operate by exerting a constant functional effect on one or a series of system elements. Forrester makes no use of gravity subsystems.

Deterministic versus Probabilistic

A deterministic model is a definate cause and effect model. A probabilistic model assigns a series of outcomes, each weighted with a definate probability, to each cause.

The models discussed here are deterministic. Considering the simplicity of these models, this is an appropriate nature for the systems. However, certain features of the models, such as the decline of businesses in the urban model, should be treated stochastically even with the models' present level of aggregation. As the models become more resolved, more system elements

will have to be treated in a probabilistic manner.

Simultanious versus Sequential

This classification distinguishes models on the basis of the manner in which their equations are solved. Simultanious models seek values for all variables at once. Sequential models evaluate system elements in a definate order.

Both social models discussed here are sequential models. Unfortunately, they lack a major feature that a sequential model structure admits very easily. This feature is time delay or, its converse, reaction time. Forrester has installed a few time delays which control perception of certain model conditions by other parts of the model. But, he has few processes in his models which sequentially contribute to flows at a time dependent rate after a major system adjustment has occurred. These flow contributions, which are usually exponentially decaying in time, constitute residual changes caused by the system adjustment.

Those reaction times which do appear in Forrester's models are arbitarily chosen. This is a crucial flaw in the models since, "Evidence from analogous (or homomorphic) systems which are adaptive and open suggests that the patterning of inter-element connections, and especially the different reaction times involved, are crucial to the understanding and modelling of system structure and behavior, including reactions with the environment." (page 388, Mc70).

As this step by step inspection of the two Forrester models

has made clear, these systems are very poorly equipped to simulate the behavior of large social aggregates. Of the time dependent models which have been developed in the past six years, Forrester's models fail to meet more criteria, make more unsupported assumptions, and have a more simplistic structure than those of Crecine or Batty. The major flaws in Forrester's work are the lack of spaciality, the lack of calibration and the intense but ambiguous analiticity of the models. For these reasons, Forrester's models cannot be considered even basic representations of the social structures they are intended to mimic and their predictive capacity is, in all probability, nil.

Changes In The Models

As the preceding critique has shown, a significant body of modeling research indicates that alterations must be made in the structure and applications of Forrester's models. As has been indicated, many adjustments are needed in the feedback systems. However, only two major changes will be proposed at this time.

The first alteration to the models centers on the structures of the models themselves. The two feedback systems must have a spacial distribution built into them. The extension of the system level variables over a two dimensional zone will simultaneously make the macroscopic aspects of the models far more microscopic while it requires the inclusion of transport and communications mechanisms. While this is not the only structural change the Forrester models should absorb, it will provide one major alter-

ation serving to make the models more faithful to the modeled structure.

The second change to the Forrester models concentrates on the treatment of the models' parameters and causal structure. The two systems must be calibrated to the observed behavior of the social structures they model. This calibration cycle will require both adjustments in the numerical values of the parameters of the systems and changes in the causal relationships in the systems. The urban model should be calibrated to two cities' historical behavior for the periods for which such data are available. The partial systems in the world system must be calibrated to the corresponding processes in the world. This calibration program is currently underway in a research project conducted by D. H. Meadows and coworkers (Me72).

I wish to emphasize that these two changes are, of themselves, only a start in what must be a continuing procedure of system additions. The two adjustments proposed are only a first step in creating more realistic social models.

Figure Caption

Figure 5.1 This Figure contains a graphic form of the Forrester World Model. Flow rates are encapsilated in pentagons. Level variables are displayed in rectangles. The information system is represented by circles and dotted lines.

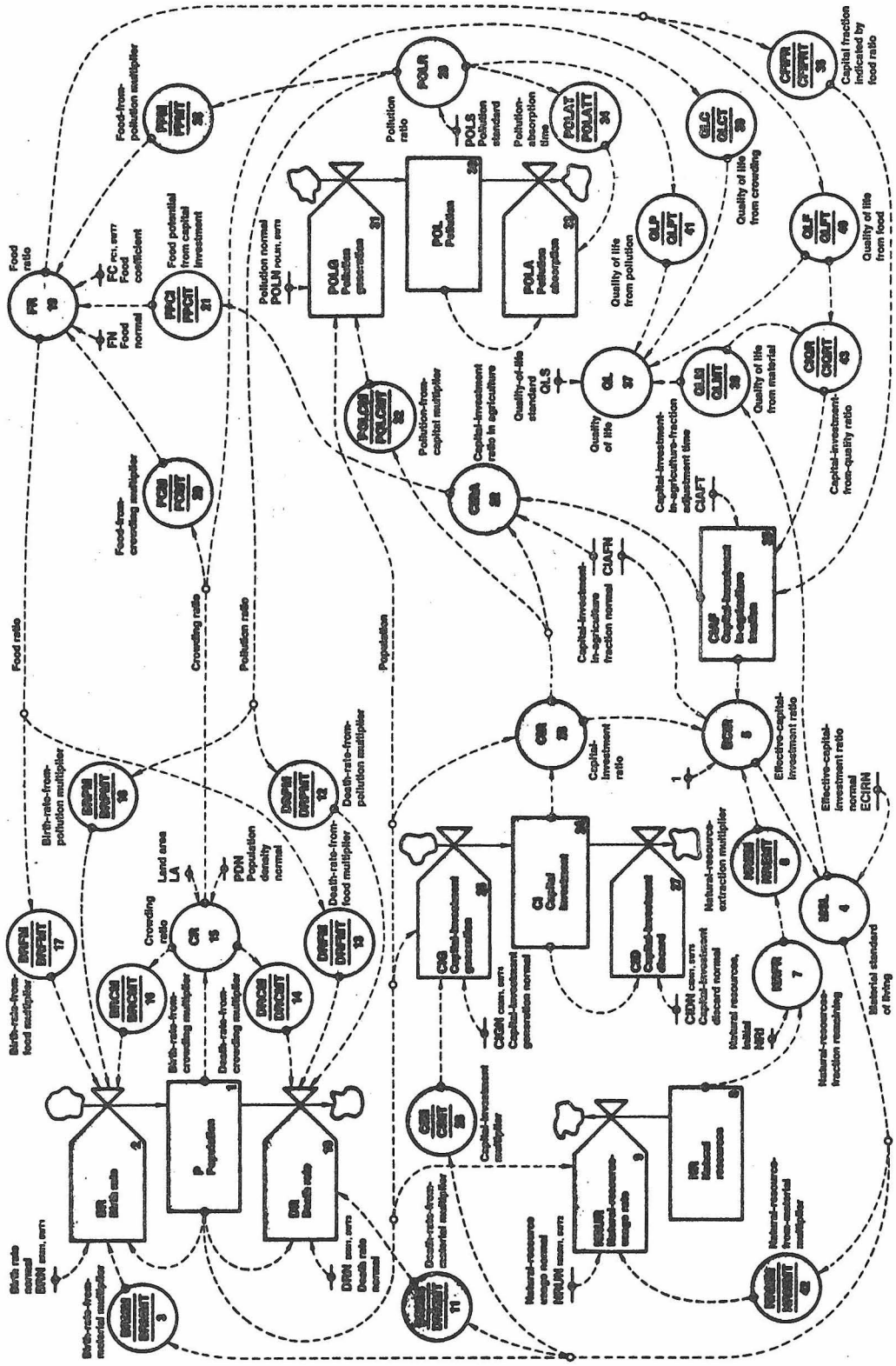

Food ratio
Crowding ratio
Pollution ratio
Population
Capital-investment ratio in agriculture
Capital-investment fraction normal CIAFN
Effective-capital-investment ratio
Effective-capital-investment ratio normal ECIRN
Material standard of living
Quality of life
Quality-of-life standard QLS
Capital-investment-in-agriculture-fraction adjustment time CIAFT
Capital-investment-from-quality ratio
Pollution normal POLN
Pollution-from-capital multiplier
Food-from-pollution multiplier
Food-from-crowding multiplier
Food potential from capital investment
Quality of life from pollution
Quality of life from crowding
Quality of life from food
Quality of life from material
Capital fraction indicated by food ratio
Pollution ratio
POLS Pollution standard
Pollution-absorption time
Land area LA
PDN Population density normal
Crowding ratio
Birth-rate-from-pollution multiplier
Birth-rate-from-food multiplier
Birth-rate-from-crowding multiplier
Death-rate-from-pollution multiplier
Death-rate-from-food multiplier
Death-rate-from-crowding multiplier
Capital-investment generation
Capital-investment discard
Capital fraction
Capital-investment multiplier
Natural-resource extraction multiplier
Natural resources, initial NRI
Natural-resource-fraction remaining
Natural-resource usage normal NRUN
Natural-resource-usage ratio
Natural-resource-from-material multiplier
Death-rate-from-material multiplier
Birth rate normal BRN
Death rate normal
Population
Pollution
Natural resources
Capital
Capital-investment in agriculture
Capital-investment in agriculture fraction
Food ratio
Quality of life
Effective-capital-investment ratio
Capital-investment ratio
Material standard of living

Figure 5.1

References

Ba71 Michael Batty, Modelling Cities As Dynamic Systems, Nature 231, 425, (1971)

Be59 Stafford Beer, Cybernetics and Management, chapter 2, page 10, John Wiley, (1959)

Be62 J. M. Bushers, Urban Social Structure, page 125, Free Press, New York, (1962)

Bo63 Richard S. Bolan, Willard B. Hansen, Neal A. Irwin, Karl H. Dieter, Planning Applications of a Simulation Model, paper prepared for the Fall Meeting, New England Section, Regional Science Association, Boston College, October (1963)

Ch60 Chicago Area Transportation Study, Final Report, Volume 2, 16-33, Chicago, (1960)

Cr68 J. P. Crecine, A Dynamic Model of Urban Structure, P-3803, Rand Corp., Santa Monica, (1968)

De64 Delaware Valley Regional Planning Commission, A Linear Interaction Model for Manufacturing Location, mimeographed document, January (1964)

Do58 J. T. Dorsey, A Communication Model for Administration, Administration Science Quarterly, 2, 307, (1958)

Fe65 J. Friedmann, Regional Development in Post-Industrial Society, Journal of the American Institute of Planners 31, 195, (1965)

Fo69 Jay W. Forrester, Urban Dynamics, The M.I.T. Press, Massachusetts, (1969)

Fo71 Jay W. Forrester, World Dynamics, Wrigth-Allen Press, Massachusetts, (1971)

Ha61 John R. Hamburg, Robert H. Sharkey, Land Use Forecast, Document #32, 610, Chicago Area Transportation Study, Chicago, (1961)

Ha67 Britton Harris, Quantitative Models of Urban Development, in Harvey S. Perloff, Lowdon Wingo, Editors, Issues in Urban Economics, page 364, Proceedings of the Conference on Urban Economics, Analysis and Policy Issues, Baltimore, John Hopkins, (1968)

Ka57 M. A. Kaplan, Balance of Power, Bipolarity and Other Models of International Systems, American Political Science Review 51, 684, (1957)

Ky67 R. L. Kyllonen, Crime Rates versus Population Density in U.S. Cities: A Model, General Systems 12, 137, (1967)

Le68 S. L. Levine, A Model of Racially Changing Neighborhoods, Socio-economic Planning Sciences 1, 477, (1968)

Le72 Letters to the Editor, Science 176, #4031, 109, (1972)

Lo64 Ira S. Lowry, A Model of Metropolis, RM-4035-RC, The Rand Corporation, Santa Monica, (1964)

Mc70 J. Brian McLaughlin, Judith N. Webster, Cybernetic and General-system Approaches to Urban and Regional Research, A Review of the Literature, Environment and Planning 2, #4, 369, (1970)

Me72 See next page.

Mi54 R. B. Mitchell, C. Rapkin, Urban Traffic; A Function of

Land Use, Columbia University Press, New York, (1954)

Se66 David R. Seidman, A Decision-Oriented Model of Urban Growth, Fourth Annual Conference of the International Federation of Operations Research Societies, Boston, September (1966)

Sh71 Martin Shubik, Book Review of World Dynamics, Science 174, #4013, 1014, (1971)

Wi48 Norbert Wiener, Cybernetics, John Wiley, New York, (1948)

Ze62 R. M. Zettel, R. R. Carll, Summary Review of Major Metropolitan Area Transportation Studies in the United States, University of California Press, Berkeley, (1962)

Me72 Donella H. Meadows, The Limits To Growth, Universe Books, New York, (1972)