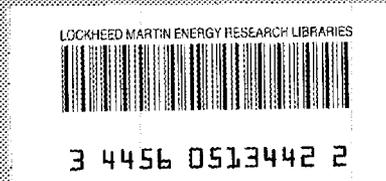


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A STUDY OF THE THREE-BODY PROBLEM IN QUANTUM MECHANICS
(Thesis)

J. H. Marble

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Submitted as a dissertation to the Graduate Council of The University of Tennessee in partial fulfillment of the requirements for the degree Doctor of Philosophy.

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J. H. Marable

Submitted as a dissertation to the Graduate Council
of The University of Tennessee in partial fulfillment of
the requirements for the degree Doctor of Philosophy.

NOVEMBER 1967

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CHAPTER I

INTRODUCTION

The quantum-mechanical three-body problem has played in the past and continues to play, as it will in the future, an important role in the development of atomic and nuclear physics.

One reason for this importance of the three-body problem is that it provides a nontrivial test of the validity of the fundamental laws of quantum mechanics. For example, the calculation by Hylleraas (1929) of the ground-state energy of the helium atom demonstrated not only the essential correctness of the atomic model but also the efficacy of the laws of quantum mechanics.

Another reason for the importance of the three-body problem is that it provides a tool for studying the forces of interaction between fundamental particles. In particular, it may be used to investigate the extent to which the two-body forces are valid for a many-body system. Thus, the study of three-body systems may help verify the results of two-body interaction studies and, at the same time, demonstrate the nature and strength of three-body forces.

Another important role played by the three-body problem is that of providing a transitional step in degree of difficulty of calculation in going from the simple two-body system to the complex many-body systems. At the same time that it provides this bridge from two-body systems to many-body systems, it may also be used as a limiting case in the general theory of many-body systems.

A three-body problem may be classified in a number of ways. One way is to classify the problem according to the particles in the system. Thus, there is the atomic three-body problem (the helium atom, for example), the molecular three-body problem (the hydrogen molecular ion), and the nuclear three-body problem (the triton). There are others, of course.

Another method of classifying three-body problems is by the physical processes involved. In particular, there are the bound states with their energy eigenvalues and the corresponding properties which may be obtained from their wave functions, and there are the unbound states which, ordinarily, are associated with collision phenomena. Some nuclear reactions, although involving many nucleons, may be viewed from the standpoint of a three-body problem. A particular example of this is deuteron stripping.

The art of calculation of the energy eigenvalues of the bound states, especially the ground states, is highly developed. However, there is still much to be done in the way of calculating the wave functions in general, and for the bound states as well as the unbound states. One of the purposes of this thesis is to develop a practical method of calculating the wave function of a three-body system in the inner region where all three particles are strongly interacting. It will be shown that such an inner wave function may be joined to an outer wave function which vanishes at large distances from the center of mass of the system in such a way as to give a good representation to the ground state of the helium atom. In order to be useful for

collision phenomena, the inner wave function will have to be joined to appropriate incoming and outgoing waves.

The first matter to be disposed of is the choice of a coordinate system. There are a number of considerations to be taken into account. Do, or should, the coordinates treat the particles in a symmetric fashion? To what extent do the coordinates separate out the motions of interest, in particular, the rotations and the translations? Are the coordinates orthogonal? Do the operators of interest (in particular, the kinetic energy, the potential energy, and the angular momenta) take on convenient forms with the coordinates chosen? To what extent is the Schroedinger equation separable in the chosen coordinates?

In an attempt to find answers to some of these questions, a method of classifying coordinates has been developed in the following Chapter II. On the basis of this classification, the form of the metric tensor is then calculated in Chapter III. Appendix B gives specific results for the two-, three-, and four-body problems.

Most workers in the past have found it convenient to separate out the center-of-mass motion, and for this reason the ordinary rectangular coordinates in the observer's frame are not suitable. On the other hand, rectangular coordinates in the center-of-mass system are redundant because they are not linearly independent. In the general N -body system, the center of mass can be separated out leaving $N-1$ cluster vectors as described in Chapter II. The coordinates of these cluster vectors form an orthogonal system of coordinates.

It is usually desirable to use coordinates which also distinguish the rotations from the other motions. Hylleraas (1928) introduced a

set of Euler angles for the rotational motion that was quite asymmetric with respect to the particles. These are the Euler angles used by Breit (1930) for his separation of the angular dependence in the two-electron problem. Derrick and Blatt (1958) discuss two ways of defining the Euler angles for the triton in a symmetric fashion. Bhatia and Temkin (1964) give a symmetric Euler-angle decomposition for the two-electron problem. Proriot (1967) generalizes this latter method to systems of three and four identical particles. In Appendix B of this thesis, the Euler angles are defined with respect to the principal axes of the system. This is one of the symmetric methods discussed by Derrick and Blatt and, for the purposes of this thesis, seems to be particularly convenient.

For the remaining three coordinates which describe the internal motion of the three-particle system, the three interparticle distances may be chosen. These form a symmetric set with respect to the three particles. These interparticle coordinates may be used to describe two-, three-, and four-body systems only, and they may not be used to describe the general N -body system. This does not destroy their usefulness for the three-body problem, however.

In the Ritz-Hylleraas variational method (Hylleraas 1929) of calculating the ground-state energy of the helium atom, asymmetric linear combinations of the interparticle distances were used. Present (1936) and Rarita and Present (1937) used these coordinates for their calculation of the triton binding energy. Again, for the helium atom, Kinoshita (1957) used a related system formed by ratios of Hylleraas coordinates.

Asymmetric linear combinations of the interparticle distances form the perimetric coordinates introduced by Coolidge and James (1937). A similar set was used by Pekeris (1958) for his extremely accurate calculation of helium atom ground-state energy. The perimetric coordinates have the advantage of having fixed ranges. Kinoshita's coordinates have this same advantage.

Gronwall (1932) showed that the introduction of the area of the three-particle triangle, along with two linear combinations of the squares of the interparticle distances, had the advantage of making the space formed by using these as coordinates conformally Euclidean.

Curtiss, Hirschfelder, and Adler (1950) introduce the lengths of the two cluster vectors and the angle between them as internal coordinates. Baker, Gammel, Hill, and Wills (1962) use the same coordinates. Luke, Meyerott, and Clendenin (1952) use two sides of the three-body triangle and the included angle as coordinates.

In Chapter II of this thesis, the classification of the internal coordinates is refined. In this way a set of coordinates for the three-body system has been found which treats all three particles symmetrically, which further distinguishes between various internal motions, and which diagonalizes the metric tensor as much as is consistent with the known failure of complete separability of the rotational motion. The classification is done for the general N-body problem, and hence, the corresponding generalization of the coordinate system should be possible. The generalization to the four-body coordinates is done in Appendix B.

Similar three-body coordinates have been found almost simultaneously and apparently independently by Gallina, Nata, Bianchi, and Viano (1962), by Kramer (1963), and by Zickendraht (1965).

After the choice of a coordinate system there remains the determination of the wave function. The usual procedure is to choose a set of functions in which to make an expansion, direct integration of the Schroedinger equation being ordinarily out of the question. The problem then reduces to determination of the coefficients of the series expansion, which is truncated at some point.

A set of functions may be found in various ways. The center-of-mass motion is always ignored, since it may be factored out of the wave function. The rotational motion is not so simply disposed of. Curtiss, Hirschfelder, and Adler (1950) show how a wave function of definite angular momentum decomposes into a sum, each term of which is a product of a rotation function and an internal function. The rotation functions associated with the orbital motion are just those functions which Wigner (1931) showed were associated with the symmetric top and which were first obtained by Reiche and Rademacher (1926) and Kronig and Rabi (1927).

In addition to the separation of the orbital motion for the triton, it is desirable to separate out the spin dependence, the I-spin dependence, the parity, and to give the symmetry classification with respect to particle interchange. Derrick and Blatt (1958) give such a classification for the triton, Clapp (1961) gives an even more complete treatment.

One of the earliest sets of internal functions, which depends on the three internal coordinates, was that chosen by Hylleraas (1929) for his Ritz variation calculation of the helium atom ground-state energy. The form of these functions is a power series in the three Hylleraas coordinates multiplied by a suitable exponential which guarantees that the function vanishes in the limit of large electron displacements as well as guaranteeing the convergence of the variation integrals. The same functions may be used for calculations of the triton binding energy as was shown by Present (1936) and Rarita and Present (1937). Coolidge and James (1937) showed that the Hylleraas form is complete in a certain sense which is sufficient for the binding energy calculation.

Kinoshita (1957) uses a more complete expansion than that of Hylleraas in that Kinoshita's series contains some terms with negative powers. Thus, Kinoshita's series includes Hylleraas's as a subseries.

Pekeris (1959) uses an expansion in a series of products of three Laguerre polynomials, each polynomial having for its argument one of the perimetric coordinates. Again, as with the Hylleraas functions and the Kinoshita functions, the series is multiplied by a suitable exponential function.

A series expansion in Legendre polynomials, the argument of which is the cosine of one of the angles of the three-particle triangle, was made by Luke, Meyerott, and Clendenin (1952). The coefficients of these polynomials are functions of two variables and must satisfy a second-order partial differential equation. Baker, Gammel, Hill, and Wills (1962) use a similar expansion.

For scattering problems, the plane wave expansions are especially useful. This is because they are so closely related to the direct physical observations as well as having nice analytical properties. They do not form a denumerable basis, however, and, hence, the expansion of the so-called internal wave functions in these functions cannot be treated by the usual method of truncating.

Delves (1960) writes the wave function in the form of a product of two spherical harmonics, the arguments of which are the angles of the spherical coordinates of the two cluster vectors, respectively. This product is multiplied by a function of the remaining two coordinates, which are the lengths of the two cluster vectors. The latter function is shown to satisfy a certain second-order partial differential equation.

Delves goes on to show that this equation is separable after a change of coordinates is made. One of these coordinates is the radius of gyration, and the other is an angle of projection. The resulting set of functions form a denumerable basis.

This set of functions is closely related to the functions studied by Zickendraht (1965) and in Chapter IV of this thesis, where the starting point is that of forming harmonic polynomials in six-dimensional space.

After the selection of the set of functions in which to expand the wave function, the actual calculations must be carried out. Bethe and Salpeter (1957) review the methods available for the calculation of the atomic three-body problem. Verde (1957) gives a review of the nuclear three-body problem.

Until recently the only method used for the calculation of the triton binding energy was the variational technique. A good example of this is the work of Pease and Feshbach (1952) in their study of the triton. Reference to earlier work may be found there.

The variational technique is of only limited usefulness for the calculation of excited states, unbound states, and wave functions in general. This was pointed out by Mitra (1962) who made one of the first successful approaches to a calculation of the triton by a method other than the variational one. His approach was made possible by the use of a separable potential. Earlier work with a very short range potential had been done by Skornyakov and Ter-Martirosyan (1956).

Aaron, Amado, and Yam (1964) used a field-theoretic approach to the three-body problem. However, their method is formally equivalent to the method of Mitra. They found a reasonable value for the triton binding energy and resolved the question of neutron-deuteron scattering lengths.

In Chapter V of this thesis an apparently novel method of calculating the wave function and energy eigenvalue of a bound state of a three-body system is developed. The method is based on an expansion of the wave function which reduces the Schroedinger equation to a set of coupled ordinary differential equations. The method does not depend on the form of the potential except insofar as the resulting wave functions may be well represented by the truncated expansion.

A generalization of two-body collision theory to three or more bodies was made by Delves (1958, 1959, 1960). He showed that by using a denumerable set of functions, the many-particle channel wave functions

were formally identical to the two-body channel wave functions.

Roskies (1966) generalized R-matrix theory to three-body systems for the restricted case for which there were no two-body interactions. He pointed out that the results of Delves were valid only for this restricted situation. Roskies discussed analytic properties of the S-matrix and gave a three-fold classification of three-body collisions: (1) two-body collisions, (2) sequential collisions, and (3) real three-body collisions.

The formal theory of the scattering of a three-particle system has been clarified by Faddeev (1960, 1961, 1962), by Lovelace (1964), and by Weinberg (1964). In the practical solution to the problem, however, there remains the difficulty associated with the multiplicity of coordinates.

CHAPTER II

THE CLASSIFICATION OF COORDINATES

In the study of systems of several particles it is both desirable and easy to separate out the motion of the center of mass from the so-called internal motions. This is accomplished by using orthogonal coordinates, three of which describe the center-of-mass motion, and the remainder of which describe the internal motions. There is a corresponding separation in the spherical harmonics and wave functions associated with the system.

It would be convenient if one could set up an orthogonal coordinate system, such as those described in Appendix A, which, in addition to being orthogonal, would have the property of separating out the rotational motions from the remaining internal motions, as is done for the center of mass.

Such a coordinate system does not exist. This fact is well known for the three-body system. Here it is shown that no such system exists for the general case of N bodies.

The following two questions then arise: (1) if a coordinate system which distinguishes the rotational motion from other motions cannot be completely orthogonal, just how orthogonal can it be, and (2) to what extent can one "peel off" the internal motions?

This and the following chapter, along with Appendix B, attempt to give answers to these two questions. In this chapter a method of classifying some of the internal motions in an invariant manner is developed.

The most general linear homogeneous transformation of the rectangular coordinates of N particles is obtained by operating on the $3N$ -dimensional vector formed by the components with an arbitrary $3N$ -by- $3N$ matrix. Usually one requires the matrix to be an element of a group. The resulting elements formed by the matrix product are the transformed coordinates or components.

Such a viewpoint which treats all the components homogeneously is often useful, especially for the construction of coordinate systems and the associated harmonic functions. From just this viewpoint the well known generalizations of ordinary spherical coordinates have been made (Morse and Feshbach 1953). An even more general expansion of the simple three-dimensional rectangular, cylindrical, and spherical coordinate systems is given in Appendix A by making use of a schematic cluster diagram. Such coordinate systems have the advantage of being orthogonal. The associated harmonics are also derived in Appendix A.

However, such transformations as the above are too general for the requirements of most physical applications. In particular, they disregard the natural physical correspondences between the components. For example, there is no correspondence between the x -component of one particle and the x -component of another particle, or between the x -component and the y -component of the same particle.

The above viewpoint can be brought into greater accord with the requirements of physics by restricting the transformation to the direct product of a spatial rotation and a linear substitution on the particles.

Accordingly, the transformation will be written in the form

$$\mathbf{x} \rightarrow \bar{\mathbf{x}} = \mathbf{R} \mathbf{x} \mathbf{U} , \quad (2.1)$$

where x is a three-by- N matrix consisting of the rectangular components (specifically, x_{ij} is the i th component of the j th particle), \bar{x} is the corresponding matrix of transformed components, R is a three-by-three orthogonal matrix specifying the rotation, and U is an N -by- N matrix specifying the linear substitution on the particles. The matrix R is chosen to be an orthogonal matrix in order to keep distance a rotational invariant. R is an element of the rotation group. At this point one requires of U only that it be an element of a group.

Under the rotation R the components of one particle transform in the same way as the components of another particle, and the components belonging to different particles are not mixed. On the other hand, the transformation induced by U causes the x -components of different particles to combine in the same way as the y - and z -components, but x -components are not mixed with y -components, only with other x -components.

It is advantageous at this point to enlarge the subgroup of rotations to the subgroup consisting of translations as well as rotations. This may be done by introducing homogeneous coordinates in the spirit of projective geometry (Graustein 1947). Instead of three nonhomogeneous (ordinary) components, x , y , and z , for each particle, there are four homogeneous coordinates, λx , λy , λz , and λ , where λ is an arbitrary nonvanishing scalar which may be different for each particle.

In order to confine the physical problem to metric geometry λ is chosen as unity, although it will be shown that a better choice would be the square root of the mass of the particle. In any case, the

ordinary nonhomogeneous coordinates are found by dividing each of the first three homogeneous coordinates by the fourth.

The use of such homogeneous coordinates allows the transformation consisting of a rotation R and a translation d to be specified by a four-by-four matrix T of the form

$$T = \begin{bmatrix} R & d \\ 0 & 1 \end{bmatrix} . \quad (2.2)$$

The corresponding transformation of the coordinate matrix is

$$r \rightarrow \bar{r} = T r U , \quad (2.3)$$

where r is of the form

$$r = \begin{bmatrix} x \\ 1 \end{bmatrix} ; \quad (2.4)$$

\bar{r} has a similar form in which the last row contains only unit elements.

For the purposes of mechanics a diagonal mass matrix is introduced,

$$m = \begin{bmatrix} m_1 & & & & \\ & m_2 & & & \\ & & m_3 & & \\ & & & \ddots & \\ & & & & m_N \end{bmatrix} . \quad (2.5)$$

Lagrangian mechanics applied to the above formalism yields the following quantities of physical interest: (1) the kinetic energy

$$K = \frac{1}{2} \text{Trace}(\dot{r}m\dot{r}') , \quad (2.6)$$

where, as usual, the dot above indicates the time derivative, and the prime denotes the transposed matrix; (2) the linear momentum

$$p = \dot{r}m , \quad (2.7)$$

where p_{ij} is the momentum conjugate to r_{ij} ; and (3) the symmetric moment-of-inertia matrix

$$M = rmr' , \quad (2.8)$$

the elements of which are the plane moments of inertia, the products of inertia, the center-of-mass coordinates, and the total mass of the system. The plane moments are the mass-weighted second moments of the rectangular components.

A generalized angular momentum matrix can also be formed by taking the anti-symmetric part of the direct product of r with p . This has been the subject of an investigation by Smith (1960).

Under a time independent transformation (which is interpreted herein to be a change in the coordinate system) r transforms as follows:

$$r \rightarrow \bar{r} = TrU . \quad (2.9)$$

There corresponds

$$m \rightarrow \bar{m} = U^{-1} m U'^{-1} , \quad (2.10)$$

$$K \rightarrow \bar{K} = K = \frac{1}{2} \text{Trace}(\dot{\bar{r}} \bar{m} \dot{\bar{r}}') , \quad (2.11)$$

$$p \rightarrow \bar{p} = TpU'^{-1} = \dot{\bar{x}} \bar{m} , \quad (2.12)$$

and

$$M \rightarrow \bar{M} = \mathbb{T} M \mathbb{T}' = \bar{r} \bar{m} \bar{r}' . \quad (2.13)$$

The transformations induced by \mathbb{T} , that is, rotations and translations, form the Euclidean group. The transformations induced by U will be called kinematic transformations, generalizing the nomenclature of Smith (1959).

A particular type of kinematic transformation is the trivial reordering transformation. For example, if initially particle 1 and particle 2 with masses m_1 and m_2 are at r_1 and r_2 respectively, after applying the reordering transformation, particle 2 and particle 1 with masses m_2 and m_1 will be at r_2 and r_1 respectively. Such a transformation may be represented by a permutation matrix, which has in each row and each column only one nonvanishing unit element.

The mass matrix m remains symmetric under an arbitrary transformation, but it does not necessarily remain diagonal. There is a special subgroup of transformations which keep the mass matrix diagonal. Such a transformation has the form

$$U = m_1^{\frac{1}{2}} O m_1^{\frac{1}{2}} , \quad (2.14)$$

where $m_1^{\frac{1}{2}}$ is the square root of the initial mass matrix before the transformation, O is an arbitrary orthogonal matrix of order N , and $m_1^{\frac{1}{2}}$ is the square root of the final transformed mass matrix. No diagonal element of m_1 may vanish.

It is now clear that the initial mass matrix may be transformed once and for all into the unit matrix I if the initial kinematic transformation is chosen to be

$$U = m^{\frac{1}{2}}, \quad (2.15)$$

and if all subsequent kinematic transformations are confined to orthogonal matrices in N dimensions.

The effect of the kinematic transformation of Equation (2.15) on the other quantities of physical interest is given by the following:

$$r \rightarrow \bar{r} = r m^{\frac{1}{2}}, \quad (2.16)$$

$$K \rightarrow \bar{K} = \frac{1}{2} \text{Trace}(\dot{\bar{r}} \dot{\bar{r}}), \quad (2.17)$$

$$p \rightarrow \bar{p} = \dot{\bar{r}}, \quad (2.18)$$

$$M \rightarrow \bar{M} = \bar{r} \bar{r}', \quad (2.19)$$

as

$$m \rightarrow \bar{m} = I. \quad (2.20)$$

It is noteworthy that an effect of the kinematic transformation $m^{\frac{1}{2}}$ is to make the fourth component of the homogeneous coordinates equal to the square root of the mass of the particle. More explicitly, the form of the transformed coordinate matrix is

$$\bar{r} = \begin{bmatrix} m_1^{\frac{1}{2}} x_1 & m_2^{\frac{1}{2}} x_2 & \dots & m_N^{\frac{1}{2}} x_N \\ m_1^{\frac{1}{2}} y_1 & m_2^{\frac{1}{2}} y_2 & \dots & m_N^{\frac{1}{2}} y_N \\ m_1^{\frac{1}{2}} z_1 & m_2^{\frac{1}{2}} z_2 & \dots & m_N^{\frac{1}{2}} z_N \\ m_1^{\frac{1}{2}} & m_2^{\frac{1}{2}} & \dots & m_N^{\frac{1}{2}} \end{bmatrix}, \quad (2.21)$$

where the elements of the matrix are given in terms of initial untransformed quantities.

The orthogonal transformation matrix

$$O = \begin{bmatrix} \left(\frac{m_2}{m_1+m_2}\right)^{\frac{1}{2}} & \left(\frac{m_1}{m_1+m_2}\right)^{\frac{1}{2}} & & & & \\ -\left(\frac{m_1}{m_1+m_2}\right)^{\frac{1}{2}} & \left(\frac{m_2}{m_1+m_2}\right)^{\frac{1}{2}} & & & & \\ & & 1 & & & \\ & & & \cdot & & \\ & & & & \cdot & \\ & & & & & \cdot \\ & & & & & & 1 \end{bmatrix} \quad (2.22)$$

applied to the right of \bar{r} gives for the first two columns of the transformed matrix

$$\begin{bmatrix} \mu_{12}^{\frac{1}{2}}(x_1 - x_2) & m_{12}^{-\frac{1}{2}}(m_1 x_1 + m_2 x_2) & \cdot & \cdot & \cdot \\ \mu_{12}^{\frac{1}{2}}(y_1 - y_2) & m_{12}^{-\frac{1}{2}}(m_1 y_1 + m_2 y_2) & \cdot & \cdot & \cdot \\ \mu_{12}^{\frac{1}{2}}(z_1 - z_2) & m_{12}^{-\frac{1}{2}}(m_1 z_1 + m_2 z_2) & \cdot & \cdot & \cdot \\ 0 & m_{12}^{\frac{1}{2}} & \cdot & \cdot & \cdot \end{bmatrix}, \quad (2.23)$$

where μ_{12} is the reduced mass of particles 1 and 2, and where m_{12} is the sum of their masses. The remaining columns are unchanged by the above transformation.

The result of a transformation such as in Equation (2.22) is to cause the fourth component of one of the column vectors to vanish, thereby indicating that this column vector represents a point on the projective plane at infinity. This vector is invariant under the translation group. After such a transformation, the original masses

m_1 and m_2 disappear completely from the formalism; only their sum remains. Of course, the masses must be remembered, or, more completely, the transformations must be remembered for a physical interpretation of the components.

The effect of the above transformation may be graphically represented as in Figure 1. The two points 1 and 2 representing particles 1 and 2 with masses m_1 and m_2 respectively, are associated with the joining line $\overline{12}$, representing the point at infinity, and with the line center l_2 , representing the center of mass of the two particles. Somewhat similar graphs have been used by Smith (1959).

Since it is associated with mass, namely, the sum of the two masses, the line center l_2 may again be used as a point in a similar transformation with another point or line center. (The distinction between real mass and reduced mass is clearly made here. It may be interesting to note, as an aside, that the latter would not be associated with any gravitational interaction.)

The transformation corresponding to a complete graph, such as shown in Figure 1, and the judicious use of reordering transformations (these are orthogonal too) cause the last row and the last column of the transformed coordinate matrix to take the form

$$\bar{r} = \begin{bmatrix} & & & & & & M^{\frac{1}{2}}X \\ & & & & & & M^{\frac{1}{2}}Y \\ & & & & & & M^{\frac{1}{2}}Z \\ & & & & & & M^{\frac{1}{2}} \\ 0 & 0 & . & . & . & 0 & M^{\frac{1}{2}} \end{bmatrix}, \quad (2.24)$$

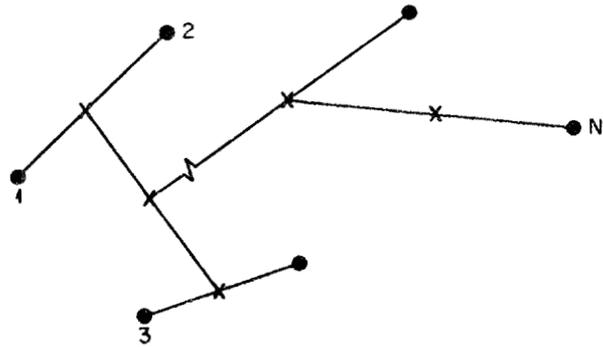
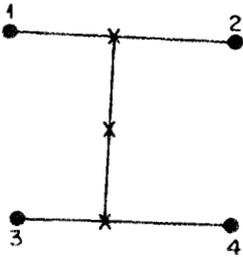
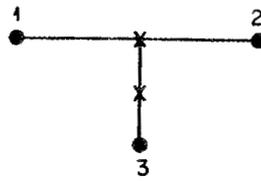
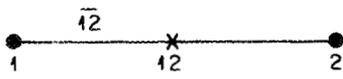


Figure 1. Graphs representing transformations to cluster coordinates for two-, three-, four-, and N-body systems.

where X , Y , and Z are the center-of-mass coordinates of the system, and where M , the total mass, is the element M_{44} of the moment-of-inertia matrix of Equation (2.19). The other elements ξ_{ij} all have the form of the square root of a reduced mass multiplying a component of a displacement vector and may be called the cluster coordinates of the system. The corresponding column vectors will be called cluster vectors.

The above reduction is carried out as far as time independent transformations can go. There are still $3N$ coordinates, but all the masses have been absorbed into the coordinates themselves; only the total mass remains. The form on the right of Equation (2.24) is invariant under the Euclidean group of translations and rotations. It is also invariant under N -dimensional orthogonal kinematic transformations O of the form

$$O = \begin{bmatrix} & & & & & 0 \\ & & & & & \cdot \\ & & O_{N-1} & & & \cdot \\ & & & & & \cdot \\ & & & & & \cdot \\ & & & & & 0 \\ 0 & \cdot & \cdot & \cdot & 0 & 1 \end{bmatrix} . \quad (2.25)$$

Again, these transformations form a subgroup.

A glance at Equation (2.19) or at Equation (2.21) reveals that scalar multiplication of the row vectors x of the coordinate matrix yields the elements of the moment-of-inertia matrix, namely, the plane moments of inertia, the products of inertia, the coordinates of the center of mass multiplied by the total mass, and the total mass itself.

This property of the row vectors is invariant under kinematic transformations with orthogonal matrices.

It is well known that there exists a Euclidean transformation T which diagonalizes the symmetric moment-of-inertia matrix M (Jeffreys and Jeffreys 1950). Such a transformation will generally be time dependent. It causes the coordinate matrix to take the form

$$\bar{r} = \begin{bmatrix} & & & & & & 0 \\ & & & & & & 0 \\ & & \bar{r}_1 & & & & 0 \\ & & & & & & 0 \\ 0 & 0 & . & . & . & 0 & M_{44}^{\frac{1}{2}} \end{bmatrix}. \quad (2.26)$$

Since the products of inertia vanish in the new coordinate system, the row vectors of the matrix \bar{r} in Equation (2.26) are orthogonal. Hence, it is readily apparent that an orthogonal kinematic transformation of the form given in Equation (2.25) exists which will give the coordinate matrix the final form

$$\bar{r} = \begin{bmatrix} 0 & . & . & . & 0 & M_{44}^{\frac{1}{2}} \rho_1 \\ 0 & . & . & . & 0 & M_{44}^{\frac{1}{2}} \rho_2 \\ 0 & . & . & . & 0 & M_{44}^{\frac{1}{2}} \rho_3 \\ 0 & . & . & . & 0 & M_{44}^{\frac{1}{2}} \end{bmatrix}. \quad (2.27)$$

This defines the ρ_i .

The values of the nonvanishing components of \bar{r} are, according to Equation (2.19), the square roots of principal plane moments of inertia. In essence, then, the coordinate matrix has been transformed into the

square root of the diagonalized moment of inertia matrix, M_o , given by

$$M_o = \begin{bmatrix} \Lambda_1 & & & \\ & \Lambda_2 & & \\ & & \Lambda_3 & \\ & & & \Lambda_4 \end{bmatrix}, \quad (2.28)$$

where $\Lambda_1, \Lambda_2, \Lambda_3$, are the principal plane moments and Λ_4 is the total mass.

The original coordinate matrix r , which gives the coordinates of the particles in the observer's reference frame, may be expressed in terms of the diagonalized moment of inertia matrix M_o by inverting the matrices used in arriving at Equation (2.27). The result is

$$r = T M_o^{-\frac{1}{2}} U_t, \quad (2.29)$$

where the subscript t on U indicates that the matrix U has been truncated to its last four rows.

The matrix T has the form

$$T = \begin{bmatrix} R & X_c \\ 0 & 1 \end{bmatrix}, \quad (2.30)$$

where R is an ordinary three-dimensional orthogonal matrix, and X_c is a vector giving the three components of the center of mass. The rotation matrix R is time dependent and depends on three coordinates, the Euler angles being examples. The center-of-mass vector X_c also depends on three coordinates, the three rectangular components themselves being examples.

Of the four nonvanishing components of the matrix $M_0^{\frac{1}{2}}$ only three may vary with time, the total mass M being kept constant. Again, three coordinates specify these three components, and, again, the components themselves may be chosen.

The form of the truncated matrix U_t is

$$U_t = O_t O_m m^{-\frac{1}{2}}, \quad (2.31)$$

where m is the diagonal mass matrix given by Equation (2.5), and O_m is an orthogonal transformation specified by the masses and a cluster graph. The time dependence of U_t is given entirely by the truncated matrix O_t which has the form

$$O_t = \begin{bmatrix} & & & & & & 0 \\ & & & & & & 0 \\ & & O_t' & & & & 0 \\ & & & & & & 0 \\ 0 & . & . & . & 0 & 0 & 1 \end{bmatrix}. \quad (2.32)$$

Here O_t' is an orthogonal matrix in $N-1$ dimensions truncated to its last three rows. There are $3(N-1)$ time dependent components with six constraints specifying the orthonormality conditions. Hence, O_t' is specified by $3N-9$ coordinates.

By using the coordinates to specify the transformations, one has a method of classifying the coordinates in an invariant manner. Thus, one may say that six external coordinates specify the transformation T , three specifying the translation and three specifying the rotation. Three size coordinates specify the diagonal moment-of-inertia matrix M_0 , and $3N-9$ internal coordinates specify the truncated kinematic transformation matrix O_t . On the basis of this classification

the internal variables and the size variables are independent of the reference frame whether it be an inertial one or not.

Even the rotational coordinates and the center-of-mass coordinates are independent tensors in the sense that their components do not mix under an arbitrary Euclidean transformation which may vary with time in an arbitrary way. That is to say, the rotation matrix in the new reference system does not depend on the center-of-mass coordinates in the old system, and, conversely, the center-of-mass coordinates in the new system do not depend on the rotational coordinates in the old system.

The single-particle system is the most trivial example. All components vanish except the center-of-mass components.

The two-particle system is characterized by three center-of-mass coordinates, only two rotation coordinates, and one size coordinate. The third rotational coordinate is lost because rotations about the line joining the two particles do not alter the configuration.

Three-particle systems are the simplest systems which have an internal coordinate according to the above classification scheme. There are, in addition to the three center-of-mass coordinates and the three rotational coordinates, two size coordinates specifying the two principal plane moments of inertial, and one internal coordinate.

The four-particle system is characterized by three rotational coordinates, a full complement of three size coordinates specifying the three principal moments, and three internal coordinates.

Another related example is the rigid body, which is characterized by having no internal coordinates, only three rotational coordinates and three translational center-of-mass coordinates. The principal moments as well as the total mass are constant parameters.

CHAPTER III

THE METRIC TENSOR FOR N-BODY COORDINATES

In the course of answering the question in the opening of Chapter II, it is necessary to calculate the metric. This is a difficult and troublesome problem unless some care is taken. The following method simplifies as far as possible the calculation, and, at the same time, shows some important structural properties of the metric tensor.

The form of the metric tensor for a system of N particles will be found using the formalism developed in the foregoing Chapter II. It will be assumed that a coordinate system has been chosen which fits the classification scheme associated with the formalism. The i th such coordinate is designated by ζ_i ; with the use of a coordinate of a particular classification, a classification label may also be appended. For example, $\zeta_{\text{rot},i}$ is the i th rotational coordinate.

The simplest method of finding the metric tensor is by elaborating the expression for the kinetic energy of Equation (2.11). The time derivative of the coordinate matrix, derived from Equation (2.29) and Equation (2.31), is

$$\dot{\mathbf{r}} = \left(\dot{\mathbf{T}}_O^{\frac{1}{2}} \mathbf{O}_t + \mathbf{T}_O^{\frac{1}{2}} \dot{\mathbf{O}}_t + \mathbf{T}_O^{\frac{1}{2}} \dot{\mathbf{O}}_t \right) \mathbf{O}_m m^{-\frac{1}{2}} . \quad (3.1)$$

Six terms are present in the resulting expression for the kinetic energy. They are as follows:

1. The external energy

$$K_{\text{ex}} = \frac{1}{2} \text{Trace}(\dot{\mathbf{T}}' \dot{\mathbf{T}} \mathbf{M}_O) . \quad (3.2)$$

2. The size energy

$$K_s = \frac{1}{2} \text{Trace}(\mathbb{T}' \mathbb{T} (\dot{M}_O^{\frac{1}{2}})^2) . \quad (3.3)$$

3. The internal energy

$$K_{in} = \frac{1}{2} \text{Trace}(M_O^{\frac{1}{2}} \mathbb{T}' \mathbb{T} M_O^{\frac{1}{2}} O_t \dot{O}_t') . \quad (3.4)$$

4. The external-internal interaction energy

$$K_{ei} = \frac{1}{2} \text{Trace}[M_O^{\frac{1}{2}} (\mathbb{T}' \dot{\mathbb{T}} - \dot{\mathbb{T}}' \mathbb{T}) M_O^{\frac{1}{2}} O_t \dot{O}_t'] . \quad (3.5)$$

5. The external-size interaction energy

$$K_{es} = \frac{1}{2} \text{Trace}[(\mathbb{T}' \dot{\mathbb{T}} + \dot{\mathbb{T}}' \mathbb{T}) M_O^{\frac{1}{2}} \dot{M}_O^{\frac{1}{2}}] . \quad (3.6)$$

6. The size-internal interaction energy

$$K_{si} = \frac{1}{2} \text{Trace}[(\dot{M}_O^{\frac{1}{2}} \mathbb{T}' \mathbb{T} M_O^{\frac{1}{2}} - M_O^{\frac{1}{2}} \mathbb{T}' \mathbb{T} \dot{M}_O^{\frac{1}{2}}) \dot{O}_t O_t'] . \quad (3.7)$$

In deriving the above six expressions, use has been made of the orthonormality properties of the truncated matrix O_t and of the diagonal character of M_O .

The expression on the right of Equation (3.7) vanishes from symmetry requirements, so that the size-internal interaction energy vanishes with it. The external-size interaction energy of Equation (3.6) vanishes also; this is seen by looking more closely at the detailed structure of the matrices. Furthermore, as is well known, the external energy decomposes into the sum of a translational energy and a rotational energy.

Use of the detailed structure of the matrices \mathbb{T} , M_O , and O_t as given in Equation (2.30), Equation (2.28), and Equation (2.32) results in the following expressions:

1. The external energies,

a) The translational energy

$$K_{tr} = \frac{1}{2} \Lambda_4 (\dot{X}_c)^2 . \quad (3.8)$$

b) The rotational energy

$$K_{rot} = \frac{1}{2} \omega' J \omega . \quad (3.9)$$

2. The size energy

$$K_s = \frac{1}{2} \dot{\rho}' \dot{\rho} . \quad (3.10)$$

3. The internal energy

$$K_{in} = \frac{1}{2} u' J u + \frac{1}{2} v' \Lambda v . \quad (3.11)$$

4. The rotation-internal energy

$$K_{ri} = \omega' E u . \quad (3.12)$$

The Λ_4 used above is just the total mass as may be recalled from its defining Equation (2.28). The matrix J has the usual moments of inertia for its diagonal elements. Explicitly,

$$J = \begin{bmatrix} \Lambda_2 + \Lambda_3 & & \\ & \Lambda_1 + \Lambda_3 & \\ & & \Lambda_1 + \Lambda_1 \end{bmatrix} . \quad (3.13)$$

Related to the matrix J is the matrix

$$E = \begin{bmatrix} \sqrt{4\Lambda_2\Lambda_3} & & \\ & \sqrt{4\Lambda_3\Lambda_1} & \\ & & \sqrt{4\Lambda_1\Lambda_2} \end{bmatrix} . \quad (3.14)$$

The column matrix ρ is given by

$$\rho = \begin{bmatrix} \rho_1 \\ \rho_2 \\ \rho_3 \end{bmatrix}, \quad (3.15)$$

where the components ρ_i , according to Equation (2.27) and Equation (2.28), satisfy the relations

$$\Lambda_i = \Lambda_i \rho_i^2 = (M_0)_{ii}. \quad (3.16)$$

The angular velocities in the body system are given by

$$\omega = \begin{bmatrix} \omega_{23} \\ \omega_{31} \\ \omega_{12} \end{bmatrix} = \begin{bmatrix} \omega_1 \\ \omega_2 \\ \omega_3 \end{bmatrix}, \quad (3.17)$$

where the components are given by

$$\omega_{ij} = (\dot{R}'R)_{ij}. \quad (3.18)$$

Just as there are angular velocities associated with the time varying rotation matrix R , so there are angular velocities associated with the time varying orthogonal matrix O . Since one row of matrix O is kept fixed according to Equation (2.25), the variation of internal coordinates apparently corresponds to the motion of a rigid body in $N-1$ dimensions. Since the only part of physical interest, however, is the truncated part of the matrix, the correspondence is rather to a rigid body of three dimensions rotating in an $N-1$ dimensional space. An analogy is a planar body moving in ordinary three-dimensional space. Some of the motions leave the plane of the body fixed, other motions tend to take the body out of its own plane.

The components of u and v of Equation (3.11) are just such angular velocities. The three angular velocity components of u , given by

$$u = \begin{bmatrix} u_{23} \\ u_{31} \\ u_{12} \end{bmatrix} = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} \quad (3.19)$$

with

$$u_{ij} = (O_t, \dot{O}'_t)_{ij} , \quad (3.20)$$

are the three components of the angular velocity which correspond to the motions which keep the three-dimensional body in its own space as it moves in $N-1$ dimensions.

The components of the angular velocity which tend to take the body out of its own space are given in the column matrix

$$v = \begin{bmatrix} v_{11} \\ v_{12} \\ \cdot \\ \cdot \\ \cdot \\ v_{1,N-4} \\ v_{21} \\ \cdot \\ \cdot \\ \cdot \\ v_{3,N-4} \end{bmatrix} = \begin{bmatrix} v_1 \\ v_2 \\ \cdot \\ \cdot \\ \cdot \\ v_{3N-12} \end{bmatrix} , \quad (3.21)$$

with the components themselves given by

$$v_{ij} = (O_{\perp} \dot{O}'_t)_{ij} . \quad (3.22)$$

$$\bar{J} = \begin{bmatrix} \frac{\Lambda_2 + \Lambda_3}{(\Lambda_2 - \Lambda)^2} & & \\ & \frac{\Lambda_3 + \Lambda_1}{(\Lambda - \Lambda_1)^2} & \\ & & \frac{\Lambda_1 + \Lambda_2}{(\Lambda_1 - \Lambda_2)^2} \end{bmatrix} \quad (3.38)$$

and

$$\bar{E} = \begin{bmatrix} \frac{\sqrt{4\Lambda_2\Lambda_3}}{(\Lambda_2 - \Lambda_3)^2} & & \\ & \frac{\sqrt{4\Lambda_3\Lambda_1}}{(\Lambda_3 - \Lambda_1)^2} & \\ & & \frac{\sqrt{4\Lambda_1\Lambda_2}}{(\Lambda_1 - \Lambda_2)^2} \end{bmatrix} \quad (3.39)$$

A result similar to this for a particular choice of coordinates for the three-body problem has been given by Derrick (1960).

The restriction to a coordinate system whose coordinates fit the classification scheme of Chapter II may be relaxed in an obvious manner. Any coordinate system may be used; the matrix \mathcal{M} remains unchanged in form, but the matrix S must be changed so that the first row contains the partial derivatives of X_{c1} with respect to each of the $3N$ coordinates, and similarly for the remaining row of S .

However, using coordinates which are invariantly classified, the metric tensor cannot be put into diagonal form except for the one- and two-body systems. This is because of the presence of the matrix E which couples the rotations with the internal motions.

Appendix B contains results of this method for calculating the metric tensor for the two-, three-, and four-body systems. Some general results are given also.

CHAPTER IV

HARMONIC FUNCTIONS FOR THE THREE-BODY SYSTEM

From this point on, this thesis will be concerned with the three-particle systems, especially those of atomic and nuclear physics.

The interaction potential between the particles is assumed to be a function depending not on the external coordinates but only on the size coordinates and the internal coordinates as classified in Chapter II. Accordingly, the wave function of the system separates into a product of two functions, a center-of-mass wave function and a so-called internal wave function. Whereas the center-of-mass wave function depends only on the center-of-mass coordinates as classified invariantly in Chapter II, the internal wave function depends on the rotational coordinates and the size coordinates as well as the internal coordinates. It is only this internal wave function of the three-particle system that will be considered here.

An important problem is that of finding a set of functions in which to expand the internal wave function, which is defined on a six-dimensional space. Eigenfunctions of the kinetic energy operator are known to be a useful set of functions in many scattering problems. These kinetic energy eigenfunctions will be used here as a basis for the expansion of the wave functions.

The problem, then, is to find these eigenfunctions as a function of the six coordinates which are invariantly classified. The particular choice of coordinates will be as chosen in Appendix B, namely, the Euler

angles α , β , and γ , the two size coordinates ρ and χ , and the single internal coordinate γ' . The angle γ' appears in the Laplacian in a form very similar to that of the Euler angle γ . (The angles α , β , and γ are the ϕ , θ , and ψ of Goldstein (1953)). These coordinates, in addition to sorting out the rotational motions, the size motions, and the internal motion, have the further advantage of treating the particles in a completely symmetric manner.

The approach considered here is similar to that of Weyl (1931) in his treatment of three-dimensional spherical harmonics. The spherical surface harmonics of order l will be constructed from the homogeneous polynomials of degree l in the rectangular coordinates of the six-dimensional space. For the use of these rectangular coordinates, the metric tensor must be the unit matrix. The rectangular coordinates may be taken to be the components of the two three-dimensional cluster vectors, that is, the cluster coordinates ξ_{ij} as defined by Equation (2.24).

It is desired to classify these energy eigenfunctions according to the total angular momentum quantum number l_0 and the corresponding azimuthal quantum number m_0 . In addition, the wave functions may be characterized by a quantum number μ which is associated with the internal motion and its coordinate γ' . There may still remain a number of solutions for a given set of these quantum numbers. The multiplicity of these solutions is derived in the following.

Delves (1960) and Zickendraht (1965) have studied the construction of such functions by the vector coupling of the two spherical harmonics associated with the two cluster vectors. This leads to

eigenfunctions of the angular momentum in a six-dimensional space. Zickendraht has found the explicit expressions for the S-, P-, and D-state functions and for some "stretched" cases of greater angular momentum.

Instead of using the rectangular components ξ_{ij} directly in the forming of the polynomials, it is convenient to form first the complex spherical basis in three dimensions. A convenient definition is

$$\underline{e}_+ = 2^{-\frac{1}{2}}(\underline{i} + i\underline{j}) , \quad (4.1)$$

$$\underline{e}_- = 2^{-\frac{1}{2}}(\underline{i} - i\underline{j}) , \quad (4.2)$$

and

$$\underline{e}_0 = \underline{k} . \quad (4.3)$$

The \underline{e}_+ , \underline{e}_- , and \underline{e}_0 form a complex orthonormal basis if the usual Hilbert space inner product is used to form the scalar product. The triplet \underline{i} , \underline{j} , \underline{k} is the familiar real orthonormal basis in the observer's system, and i is the imaginary root of -1 .

A vector in the six-dimensional space may now be specified by the six real rectangular cluster coordinates ξ_{ij} or by the three complex components Ω_+ , Ω_0 , and Ω_- . These two sets of coordinates are related by

$$\underline{\xi}_1 + i\underline{\xi}_2 = \Omega_- \underline{e}_- + \Omega_0 \underline{e}_0 + \Omega_+ \underline{e}_+ , \quad (4.4)$$

where $\underline{\xi}_1$ and $\underline{\xi}_2$ are the two cluster vectors defined by the first two rows respectively of the matrix on the right of Equation (2.24).

As in Equation (B.29) of Appendix B, the cluster coordinates may be related to the invariantly classified coordinates by a matrix

equation, namely:

$$(\underline{\xi}_1 \ \underline{\xi}_2) = \begin{bmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \\ R_{31} & R_{32} \end{bmatrix} \begin{bmatrix} \rho \cos \chi & \\ & \rho \sin \chi \end{bmatrix} \begin{bmatrix} \cos \gamma' & -\sin \gamma' \\ \sin \gamma' & \cos \gamma' \end{bmatrix}. \quad (4.5)$$

The combination of Equation (4.4) and Equation (4.5) leads to the following expressions for the complex components:

$$\Omega_0 = -i\rho 2^{-\frac{1}{2}} \exp(i\gamma') \sin \beta [\cos(\chi + \frac{\pi}{4}) \exp(i\gamma) - \cos(\chi - \frac{\pi}{4}) \exp(-i\gamma)], \quad (4.6)$$

and

$$\begin{aligned} \Omega_{\pm} = \frac{1}{2} \rho \exp(i\gamma' \mp i\alpha) & [(1 \mp \cos \beta) \cos(\chi + \frac{\pi}{4}) \exp(i\gamma) \\ & + (1 \pm \cos \beta) \cos(\chi - \frac{\pi}{4}) \exp(-i\gamma)]. \end{aligned} \quad (4.7)$$

This is a vector of magnitude given by

$$|\Omega|^2 = \Omega_0 \Omega_0^* + \Omega_+ \Omega_+^* + \Omega_- \Omega_-^* = \rho^2. \quad (4.8)$$

A homogeneous polynomial Y of degree ℓ may now be formed as follows:

$$Y = \sum_{a+b+c+d+e+f=\ell} A(a,b,c,d,e,f) (\Omega_+^*)^a (\Omega_-)^b (\Omega_-^*)^c (\Omega_+)^d (\Omega_0^*)^e (\Omega_0)^f. \quad (4.9)$$

The six indices of summation must all be non-negative. This polynomial Y will be a surface harmonic of order ℓ if the radius ρ is chosen to be unity and if the polynomial satisfies Laplace's equation in six

dimensions

$$\nabla^2 Y = 0 , \quad (4.10)$$

where ∇^2 is the Laplacian operator, which takes on the form

$$\nabla^2 = 4 \left(\frac{\partial^2}{\partial \Omega_+ \partial \Omega_+^*} + \frac{\partial^2}{\partial \Omega_- \partial \Omega_-^*} + \frac{\partial^2}{\partial \Omega_0 \partial \Omega_0^*} \right) . \quad (4.11)$$

It follows that the coefficients $A(a,b,c,d,e,f)$ must satisfy the requirement

$$\begin{aligned} (a+1)(d+1) A(a+1,b,c,d+1,e,f) + (b+1)(c+1) A(a,b+1,c+1,d,e,f) \\ + (e+1)(f+1) A(a,b,c,d,e+1,f+1) = 0 , \end{aligned} \quad (4.12)$$

if Y is to be a solution to Laplace's equation.

This functional relation (4.12) which the coefficients A must satisfy relates only those coefficients for which the following differences are fixed:

$$\delta_1 = d - a , \quad (4.13)$$

$$\delta_2 = b - c , \quad (4.14)$$

and

$$\delta_3 = f - e . \quad (4.15)$$

Hence, for any given harmonic these three differences may be assumed to be constants.

Each coefficient A may now be considered a function of only three of the summation indices, a , c , and e , instead of all six.

Equation (4.12) correspondingly becomes

$$\begin{aligned}
& (a+1)(a+1+\delta_1) A(a+1, c, e) + (c+1)(c+1+\delta_2) A(a, c+1, e) \\
& + (e+1)(e+1+\delta_3) A(a, c, e+1) = 0 .
\end{aligned} \tag{4.16}$$

This Equation (4.16) relates the three values of $A(a, c, e)$ at the points of a darkened triangle which lies in the plane

$$a + c + e = \frac{1}{2}[\ell - (\delta_1 + \delta_2 + \delta_3)] , \tag{4.17}$$

as shown in Figure 2. Not all of the darkened triangles on the simplex may be used, however. For in addition to the constraints

$$a \geq 0 , \tag{4.18}$$

$$c \geq 0 , \tag{4.19}$$

$$e \geq 0 , \tag{4.20}$$

there are also the constraints

$$b = c + \delta_2 \geq 0 , \tag{4.21}$$

$$d = a + \delta_1 \geq 0 , \tag{4.22}$$

and

$$f = e + \delta_3 \geq 0 . \tag{4.23}$$

The above six constraints may be combined into the following three:

$$a \geq a_{\min} = \max(0, -\delta_1) = \frac{1}{2}(-\delta_1 + |\delta_1|) , \tag{4.24}$$

$$c \geq c_{\min} = \max(0, -\delta_2) = \frac{1}{2}(-\delta_2 + |\delta_2|) , \tag{4.25}$$

and

$$e \geq e_{\min} = \max(0, -\delta_3) = \frac{1}{2}(-\delta_3 + |\delta_3|) . \tag{4.26}$$

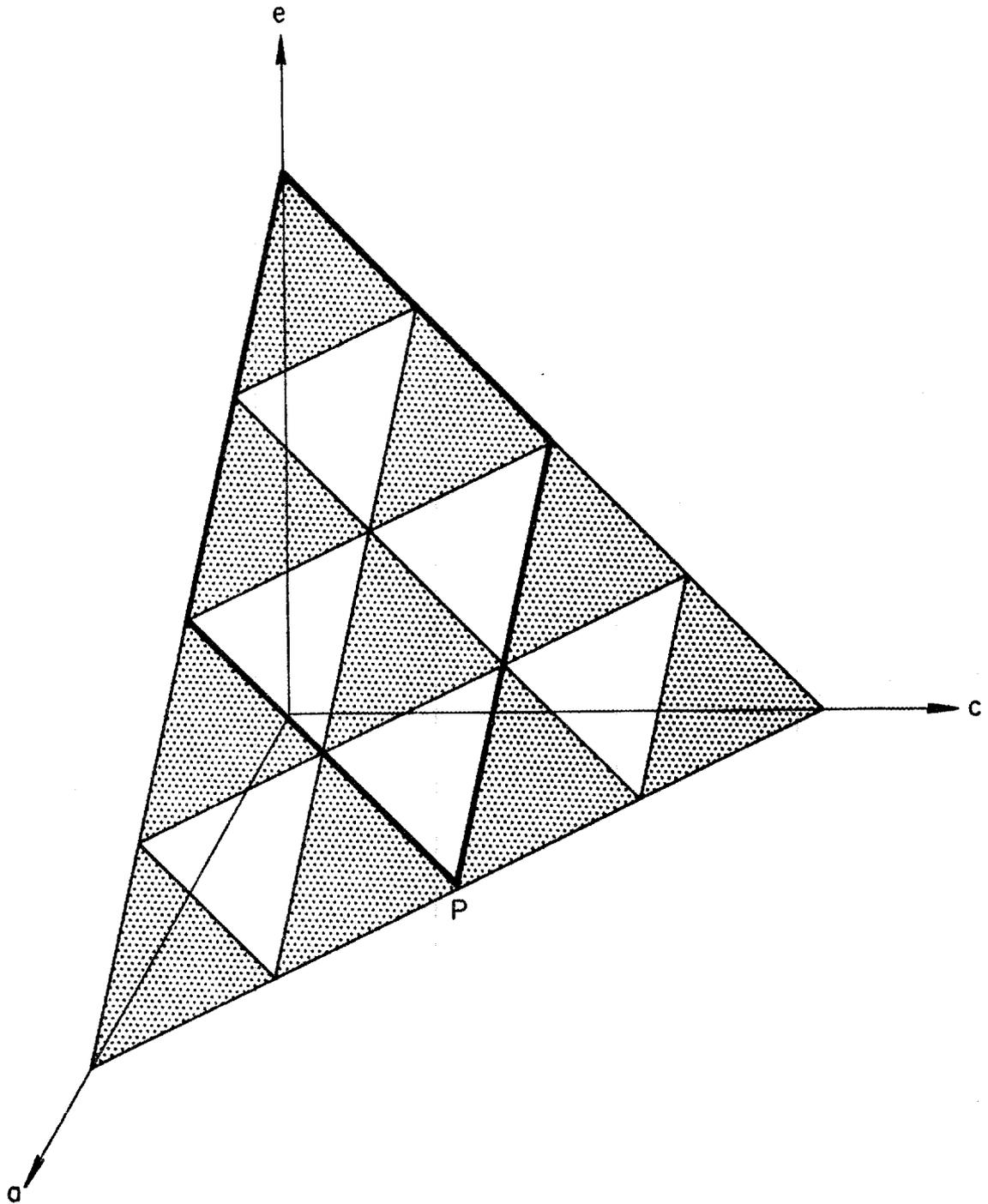


Figure 2. The darkened triangles on the vertices of which the coefficients A are related. In this example a_{\min} , c_{\min} , and e_{\min} are assumed to vanish.

The key to the solution for the coefficients A is found by observing that to each darkened triangle there corresponds an equation relating the three vertices, whereas a value for A is required at each vertex. There is a one-to-one correspondence between each triangle and its upper vertex, thus leaving the lower vertices of the lower line of triangles as points on which the values of A may be chosen independently.

If all but one of the A 's on the lower line are assumed to vanish, then the solution for the coefficients is seen to vanish everywhere except in a diamond-shaped region with bounds parallel to the sides of the simplex. Thus, in Figure 2, if the coefficients are chosen to vanish at all points in the a - c plane except at point P , then the solution vanishes everywhere except in the region surrounded by the darkened line. There are, of course, other ways of specifying the independent parameters, but any solution will be a linear combination of those found here.

It is not difficult to verify that the solution for the coefficients for such a choice of parameters is given by the following:

$$A(a, c, e) = \frac{(-1)^e (e - e_{\min})!}{a!c!(c+\delta_2)!(a+\delta_1)!e!(e+\delta_3)!(a_0-a)!(c_0-c)!}, \quad (4.27)$$

where a_0 , c_0 , and e_{\min} define the point P at which the solution does not vanish. This triplet, a_0 , c_0 , and e_{\min} , must satisfy the Equation (4.17) of the plane, namely:

$$a_0 + c_0 + e_{\min} = \frac{1}{2}[\ell - (\delta_1 + \delta_2 + \delta_3)]. \quad (4.28)$$

The spherical surface harmonics may thus be completely specified by the five parameters l , δ_1 , δ_2 , δ_3 , and a_0 . The ranges of the parameters are as follows:

$$l = 0, 1, 2, 3, \dots, \quad (4.29)$$

$$\delta_i = -l, -l + 1, \dots, l - 1, l, \quad (4.30)$$

with the restriction that

$$|\delta_1| + |\delta_2| + |\delta_3| = l, l - 2, l - 4, \dots, \quad (4.31)$$

and

$$a_0 = \frac{1}{2}(-\delta_1 + |\delta_1|), \dots, \frac{1}{2}(l - \delta_1 - |\delta_2| - |\delta_3|). \quad (4.32)$$

The largest value of a_0 given above in Equation (4.32) may be combined with the minimum value a_{\min} given by Equation (4.24) to yield the number of harmonics $N_{l\delta}$ associated with the order and the triplet $(\delta_1, \delta_2, \delta_3)$. The number of harmonics is

$$N_{l\delta} = 1 + \frac{1}{2}(l - |\delta_1| - |\delta_2| - |\delta_3|). \quad (4.33)$$

The effect of an infinitesimal rotation of the observer's coordinate system will not change the degree of the polynomial. Hence, l is an invariant. The other parameters, δ_1 , δ_2 , δ_3 , and a_0 , are not invariant under rotations.

The effect of such a rotation may be calculated in the following way. First, the effect of the transformation on the cluster coordinates is calculated, then the corresponding effect using the complex spherical basis, and finally the effect on the terms of the polynomial itself.

An infinitesimal rotation R acting on the rectangular cluster coordinates ξ_{ij} is given by

$$\xi \rightarrow (R\xi) = (I + \omega) \xi . \quad (4.34)$$

I is the unit matrix, and ω is given in terms of the infinitesimal rotation with components ω_1 , ω_2 , and ω_3 by the following matrix:

$$\omega = \begin{bmatrix} 0 & \omega_3 & -\omega_2 \\ -\omega_3 & 0 & \omega_1 \\ \omega_2 & -\omega_1 & 0 \end{bmatrix} . \quad (4.35)$$

The corresponding effect on the components Ω_- , Ω_0 , and Ω_+ in the spherical basis may be calculated from Equation (4.4), Equation (4.34), and Equation (4.35) to obtain

$$\Omega \rightarrow (R\Omega) = \begin{bmatrix} (1 - i\omega_3) \Omega_- + 2^{-\frac{1}{2}}(-\omega_2 + i\omega_1) \Omega_0 \\ \Omega_0 + 2^{-\frac{1}{2}}(\omega_2 + i\omega_1)\Omega_- + 2^{-\frac{1}{2}}(\omega_2 - i\omega_1) \Omega_+ \\ (1 + i\omega_3) \Omega_+ + 2^{-\frac{1}{2}}(-\omega_2 - i\omega_1) \Omega_0 \end{bmatrix} . \quad (4.36)$$

The powers of the spherical components which appear in the terms of the harmonic Y on the right of Equation (4.9) then undergo the following transformations:

$$(\Omega_+^*)^a = (\Omega_+^*)^{a-1} [\Omega_+^* + i\omega_1 2^{-\frac{1}{2}} a \Omega_0^* - \omega_2 2^{-\frac{1}{2}} a \Omega_0^* - i\omega_3 a \Omega_+^*] , \quad (4.37)$$

$$(\Omega_-^*)^b = (\Omega_-^*)^{b-1} [\Omega_-^* + i\omega_1 2^{-\frac{1}{2}} b \Omega_0^* - \omega_2 2^{-\frac{1}{2}} b \Omega_0^* - i\omega_3 b \Omega_-^*] , \quad (4.38)$$

$$(\Omega_-^*)^c = (\Omega_-^*)^{c-1} [\Omega_-^* + i\omega_1 2^{-\frac{1}{2}} c \Omega_0^* - \omega_2 2^{-\frac{1}{2}} c \Omega_0^* + i\omega_3 c \Omega_-^*] , \quad (4.39)$$

$$(\Omega_+)^d = (\Omega_+)^{d-1} [\Omega_+ - i\omega_1 2^{-\frac{1}{2}} d \Omega_0 - \omega_2 2^{-\frac{1}{2}} d \Omega_0 + i\omega_3 d \Omega_+] , \quad (4.40)$$

$$(\Omega_0^*)^e = (\Omega_0^*)^{e-1} [\Omega_0^* - i\omega_1 2^{-\frac{1}{2}} e (\Omega_+^* - \Omega_-^*) + \omega_2 2^{-\frac{1}{2}} e (\Omega_+^* + \Omega_-^*)] , \quad (4.41)$$

$$(\Omega_0)^f = (\Omega_0)^{f-1} [\Omega_0 - i\omega_1 2^{-\frac{1}{2}} f (\Omega_+ - \Omega_-) + \omega_2 2^{-\frac{1}{2}} f (\Omega_+ + \Omega_-)] . \quad (4.42)$$

Only the first order terms have been retained.

It may be seen that the component ω_3 leads to no new harmonics. That is, the harmonics given by Equation (4.9) are invariant with respect to rotations about the z-axis. On the other hand, the components ω_1 and ω_2 lead to two new harmonic functions. The linear combinations $(\omega_1 + i\omega_2)$ and $(\omega_1 - i\omega_2)$ are associated with the harmonics produced by the familiar "raising" and "lowering" operators of angular momentum theory (Rose 1957). According to Equation (4.37) through Equation (4.42), the harmonics produced are given by the following two linear combinations of coefficients:

$$\begin{aligned} A_+(a, c, e; \delta_1, \delta_2, \delta_3) &= (a+1) A(a+1, c, e-1; \delta_1-1, \delta_2, \delta_3+1) \\ &\quad - (e+\delta_3+1) A(a, c, e; \delta_1-1, \delta_2, \delta_3+1) \\ &\quad + (c+\delta_2+1) A(a, c, e; \delta_1, \delta_2+1, \delta_3-1) \\ &\quad - (e+f) A(a, c-1, e+1; \delta_2+1, \delta_3-1) \end{aligned} \quad (4.43)$$

and

$$\begin{aligned} A_-(a, c, e; \delta_1, \delta_2, \delta_3) &= (c+1) A(a, c+1, e-1; \delta_1, \delta_2-1, \delta_3+1) \\ &\quad - (e+\delta_3+1) A(a, c, e; \delta_1, \delta_2-1, \delta_3+1) \\ &\quad + (a+\delta_1+1) A(a, c, e; \delta_1+1, \delta_2, \delta_3-1) \\ &\quad - (e+1) A(a-1, c, e+1; \delta_1+1, \delta_2, \delta_3-1) . \end{aligned} \quad (4.44)$$

Thus, if a harmonic function is given in terms of its coefficients $A(a, c, e; \delta_1, \delta_2, \delta_3)$, then the coefficients of two new harmonic functions are defined by Equation (4.43) and Equation (4.44) respectively.

The coefficients defined by Equation (4.27) are assumed to vanish except for a unique set of values for the triplet $(\delta_1, \delta_2, \delta_3)$. The associated harmonics produced by the "raising" and "lowering" operators from the harmonic of Equation (4.27) each have two sets of values for the triplet $(\delta_1, \delta_2, \delta_3)$, as may be seen from Equation (4.43) and Equation (4.44). These two equations also show, however, that the sum

$$\delta_1 + \delta_2 + \delta_3 = \mu = \ell - 2n \quad (4.45)$$

is invariant under the rotation group. The second equality follows from Equation (4.17) and defines n .

Furthermore, Equations (4.43) and (4.44) show that each harmonic may be characterized by a constant difference

$$m_0 = \delta_1 - \delta_2 . \quad (4.46)$$

The effect of the "raising" operator is to increase m_0 by unity and the effect of the "lowering" operator is to decrease m_0 by unity. It therefore seems reasonable that m_0 is the azimuthal quantum number for the orbital angular momentum, and it will be seen that this interpretation is correct.

The classification of the harmonics is usually desired with respect to the rotation subgroup. This classification will be characterized by ℓ and μ since they are invariants. For a given ℓ the triplet $(\delta_1, \delta_2, \delta_3)$ is confined to the interior of the equilateral octahedron

$$|\delta_1| + |\delta_2| + |\delta_3| \leq l, \quad (4.47)$$

according to Equation (4.31). This is shown in Figure 3. Also shown is the intersection of this octahedron with the plane of Equation (4.45) characterized by constant μ . On this plane of intersection may be seen the lines of constant m_0 and the lines formed by the planes of the coordinate axes.

At each point in the plane of constant μ the number of harmonics is given by Equation (4.33). In particular, at each point on the surface of the octahedron there is exactly one harmonic. Inside the octahedron, the form of the absolute magnitudes of Equation (4.33) depends on the octant. Not more than seven octants appear in any one cross section characterized by μ . The number of harmonic solutions as given by Equation (4.33) according to the octant is given in Table I.

For the particular case that $|\mu|$ is equal to l , the cross section of Figure 3 reduces to a triangle. Since all these points lie on the surface of the octahedron, there is one harmonic at each point. There is accordingly one multiplet of $(2l_0 + 1)$ harmonics for each value of the orbital angular momentum quantum number with the following allowed values,

$$l_0 = l, l - 2, l - 4, \dots \quad (4.48)$$

For the other cases in which $|\mu|$ is not equal to the order l , the number of harmonics for each value of μ and m_0 may be found by summing arithmetic series. The difference between the number of harmonics associated with a given value m_0 and the number associated with $m_0 + 1$ gives the number of multiplets for the orbital angular momentum

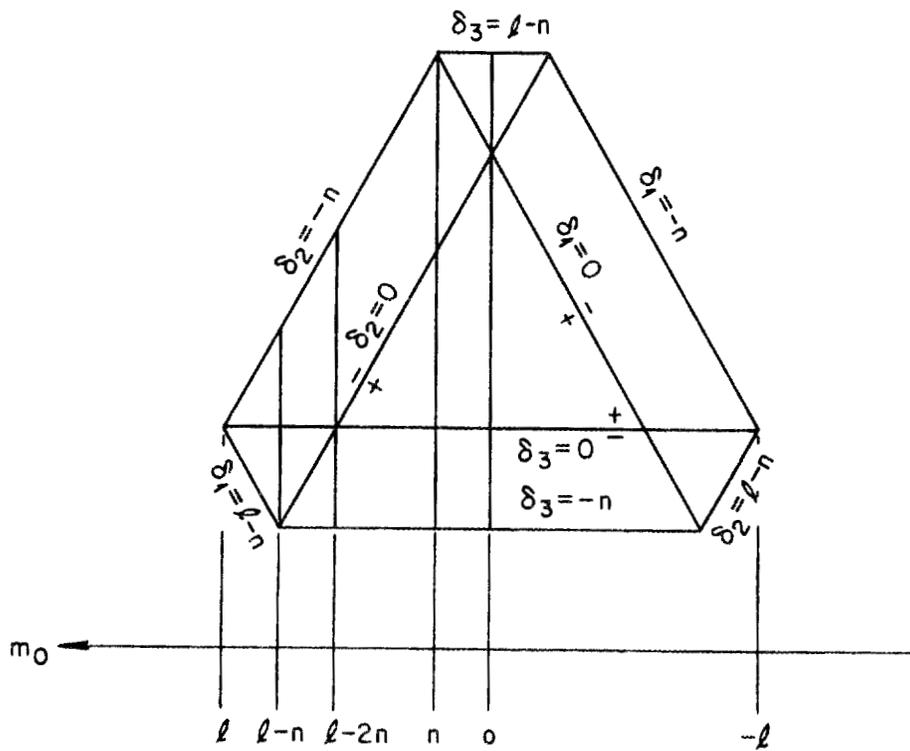
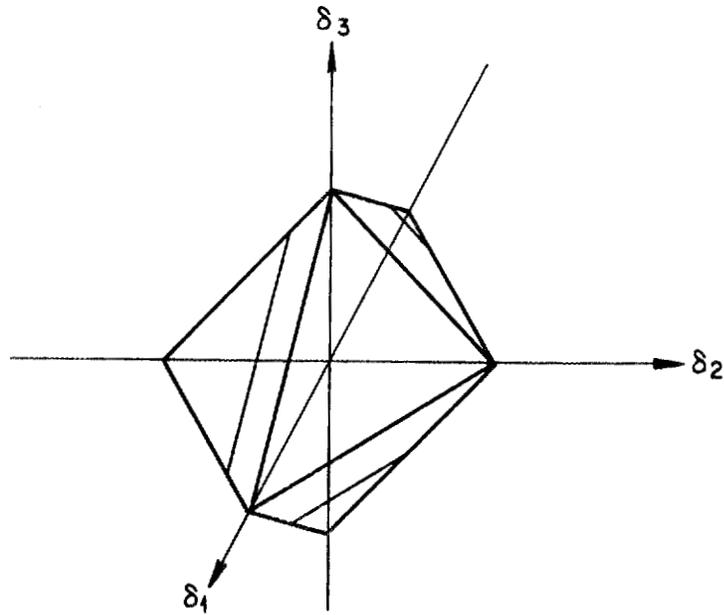


Figure 3. The equilateral octahedron $|\delta_1| + |\delta_2| + |\delta_3| = l$ and its cross section in the plane $\delta_1 + \delta_2 + \delta_3 = l - 2n$.

TABLE I
 NUMBER OF HARMONICS AT EACH POINT IN
 THE PLANE $\delta_1 + \delta_2 + \delta_3 = l - 2n$
 ACCORDING TO THE OCTANT

Octant	Number of Harmonics
+ + +	$l + n$
+ + -	$l + n + \delta_3$
+ - +	$l + n + \delta_2$
+ - -	$l + l - n - \delta_1$
- + +	$l + n + \delta_1$
- + -	$l + l - n - \delta_2$
- - +	$l + l - n - \delta_3$
- - -	$l + l - n$

quantum number l_0 equal to the value m_0 . The results of such calculations are given in Table II. These results agree with those of Zickendraht (1965), who, however, was unable to prove his results.

The harmonic functions associated with a given value of μ , l_0 , and m_0 may be calculated by starting out with the stretched case for which l_0 just equals the order of the harmonic l . By successively applying the "lowering" operator through the use of Equation (4.44) and by choosing the right linear combinations at each step, one may eventually find the harmonic desired. This method is not yet practical.

The surface harmonics may be found explicitly by another method. If the expressions for the spherical components given in Equation (4.6) and Equation (4.7) are inserted into the expression for the harmonic polynomial on the right of Equation (4.9), then, after liberal use of the binomial expansion, the result is

$$\begin{aligned}
 Y = \exp(i\gamma'\mu) \exp(-i\alpha m_0) \sum_{m'_0} \exp(-i\gamma m'_0) \\
 \sum_r \left[\cos\left(\chi + \frac{\pi}{4}\right) \right]^{(2r+\frac{1}{2}(\mu-m'_0))} \left[\cos\left(\chi - \frac{\pi}{4}\right) \right]^{(-2r-\frac{1}{2}(\mu-m'_0))} \\
 \sum_s C \left(\sin \frac{1}{2} \beta\right)^{(\ell+m_0+2s)} \left(\cos \frac{1}{2} \beta\right)^{(\ell-m_0-2s)}. \quad (4.49)
 \end{aligned}$$

It is thus revealed that the parameter μ is an eigenvalue associated with the internal angular coordinate γ' and that m_0 really is the azimuthal quantum number. The other two eigenvalues, which may be taken to be δ_z and a_0 , are hidden in the coefficients C , which are given by the following:

TABLE II
 THE NUMBER OF MULTIPLETS FOR A GIVEN SET
 OF EIGENVALUES l , μ , AND l_0

Region	Even $l - l_0$	Odd $l - l_0$
$l - n \leq l_0 \leq l$	$1 + \frac{l - l_0}{2}$	$\frac{1 + l - l_0}{2}$
$n \leq l_0 < l - n$	$1 + \left[\frac{n}{2} \right]$	$\left[\frac{n + 1}{2} \right]$
$0 \leq l_0 < n$		
a) Even n	$1 + \left[\frac{l_0}{2} \right]$	$\left[\frac{l_0}{2} \right]$
b) Odd n	$\left[\frac{1 + l_0}{2} \right]$	$\left[\frac{1 + l_0}{2} \right]$

NOTE: The square brackets mean the integral part of the quantity inside is to be taken. This table is for $\mu = l - 2n \geq 0$. To obtain the number of multiplets for negative μ , replace n by $l - n$ in the above table.

$$c = 2^{\frac{1}{2}\delta_3} (-i)^{\delta_3} \sum_{\substack{a+c+e=\frac{1}{2}(\ell-\mu) \\ i+k+n=r \\ j+\lambda+\nu=\frac{1}{2}(\ell+m'_0)-r \\ i+j-k-\lambda=s}} \frac{(-1)^e 2^e (e - e_{\min})!}{i!j!k!\lambda!n!\nu!(a-i)!(c+\delta_2-j)!(c-k)!} \cdot \frac{(a+\delta_1-\lambda)!(e-n)!(e+\delta_3-\nu)!}{(a_0-a)!(\frac{1}{2}(\ell-\mu)-a_0-e_{\min}-c)!} \quad (4.50)$$

This multiple sum in Equation (4.50) is taken over all positive values of the indices subject to the constraints shown under the summation sigma. The reduction to a sum over five indices is trivial. It is likely that even further reduction of the indices may be made.

The harmonic thus developed is not characterized by a fixed value of the orbital angular momentum ℓ_0 . It can, however, be expanded into a sum of such terms, each of which is characterized by a value of ℓ_0 . This is done by taking from each term on the right of Equation (4.50) that factor which depends on the Euler angle β and expanding it as a series in the rotation functions $d_{m_0 m}^{\ell_0}(\beta)$. The resulting coefficients which appear in the harmonic are even more complex than those given by Equation (4.50). It may well be possible that these multiple sums can be reduced to simpler forms.

The results presented in this chapter of these investigations into the properties of the harmonic functions are not needed in the following chapters.

CHAPTER V

THE APPLICATION OF THE METHOD

In order to apply the method developed in the foregoing chapters and to test its usefulness as a calculational tool, a FORTRAN program has been written for the CDC-1604 computer

The program has been limited in two respects. First, the orbital angular momentum is restricted so as to include S states only. There are a number of reasons for this restriction, the foremost being that of simplicity. (At present, the forms of the harmonics have been worked out by Zickendraht (1965) for the S, P, and D states only, so that, at most, only three values of the angular momentum could be used.) With this restriction, the program is able to calculate the ground state and some of the excited states of a three-particle atomic system and the most important contribution to the ground state of a nuclear system.

The second restriction concerns the potential function. It may be quite general in the form of its spatial dependence (it is specified in a subroutine), but in the initial version of the program there may be no dependence on internal degrees of freedom, such as spin. The restriction is of little concern for the atomic systems, but is a serious limitation on the calculation of nuclear systems. The potential does not need to be a sum of two-body potentials.

In addition to these two restrictions, the program is directed toward the calculation of bound-state wave functions and the corresponding

energy eigenvalues. The program will also calculate the wave function at an arbitrary energy, at least in the neighborhood of the origin. Generally, however, a large number of harmonics is needed for a valid expansion of the wave function of an unbound system at large distances from the center of mass of the system.

Of course, the principal motivation for the development of the method is to calculate scattering phenomena. However, the bound system has been chosen here because it can more readily demonstrate the capabilities of the method.

The helium atom has been chosen in particular because it provides a good first test of the method. The Coulomb potential is not complicated by spin dependence, and, moreover, the well-known results for the helium atom provide a reliable check on the answers calculated by the method.

In the following, the wave function and the potential energy will each be expanded in a series of harmonics. The Clebsch-Gordan series will be applied to find the corresponding series expansion for the product of the potential energy and the wave function. The Schroedinger equation reduces to a set of ordinary second-order differential equations coupling the harmonic coefficients of the wave function. This equation may be integrated by simple numerical techniques.

A complete set of solutions satisfying the inner boundary conditions is integrated outward to a match point. Similarly, a complete set of solutions satisfying boundary conditions at a distant point (representing infinity) is integrated inward to the match point. According to the discrepancy in the two sets of solutions at the match

point, a new solution made up of linear combinations of the old is chosen so as to be as smooth as possible. By integrating the square of this new wave function, a new estimate of the eigenenergy may be made.

The Schroedinger wave equation for the three particles is

$$-\frac{\hbar^2}{2} \nabla^2 \psi + V\psi = E\psi . \quad (5.1)$$

The total mass of the system is assumed to be unity throughout this chapter. The symbol ∇^2 represents the Laplacian operator in six dimensions and, for S states, is given by

$$\nabla^2 = \rho^{-5/2} \frac{\partial^2}{\partial \rho^2} \rho^{5/2} + \rho^{-2} (\Lambda - 15/4) , \quad (5.2)$$

where

$$\Lambda = \frac{16}{\sin 4\chi} \frac{\partial}{\partial(4\chi)} \sin 4\chi \frac{\partial}{\partial(4\chi)} + \frac{2}{1 + \cos 4\chi} \frac{\partial^2}{\partial \gamma'^2} . \quad (5.3)$$

The coordinates are those described in Appendix B. The variable ρ has the range $(0, \infty)$; the variable χ has the range $(0, \pi/4)$, and the variable γ' has the range $(0, \pi)$.

The wave function is now expanded in the surface harmonics of Chapter IV. The expansion is

$$\psi(\rho, \chi, \gamma') = \sum_{\ell\mu} \psi_{\ell\mu}(\rho) Y_{\ell\mu}(\chi, \gamma') . \quad (5.4)$$

Only the S-state surface harmonics appear in the series. From Table II, page 53, it is seen that there is one S-state harmonic of even order ℓ for values of μ differing from ℓ by four.

The harmonics are most easily found, perhaps, by finding the eigenfunctions of the operator of Equation (5.3). The solution is

separable in the following form

$$Y_{\ell\mu}(\chi, \gamma') = A_{\ell\mu}(\chi) f_{\mu}(\gamma') . \quad (5.5)$$

The boundary conditions may be obtained from considerations of the eight three-particle configurations which are mutually related to one another by a rotation that carries the principal axes into themselves. For an S-state the boundary condition with regard to the internal variable γ' becomes

$$f_{\mu}(\pi) = f_{\mu}(0) . \quad (5.6)$$

The separability assumption of Equation (5.5) inserted into the eigenvalue equation arising from the operator of Equation (5.3) with the boundary condition Equation (5.6) leads to the solution

$$f(\gamma') = \exp(i2\nu\gamma') \quad \text{for } \nu = 0, \pm 1, \pm 2, \dots . \quad (5.7)$$

This is just what was predicted, of course, from Table II, page 53.

The ν appearing in Equation (5.7) is just half the value of μ , which must be even.

In a similar way, the functions $A_{\ell\mu}(\chi)$ may be found. For S states the boundary conditions are

$$\frac{d}{d\chi} A_{\ell\mu}(0) = 0 , \quad (5.8)$$

and

$$\frac{d}{d\chi} A_{\ell\mu}(\pi/4) = 0 \quad \text{for even } \nu , \quad (5.9)$$

or

$$A_{\ell\mu}(\pi/4) = 0 \quad \text{for odd } \nu . \quad (5.10)$$

The equation to be satisfied for a harmonic of order ℓ is

$$\left[\frac{16}{\sin 4X} \frac{d}{d(4X)} \sin 4X \frac{d}{d(4X)} - \frac{8\nu^2}{1 - \cos 4X} + \ell(\ell + 4) \right] A_{\ell\mu}(X) = 0. \quad (5.11)$$

The solution is found to be

$$\begin{aligned} A_{\ell\mu}(X) &= (\cos 2X)^\nu {}_2F_1(-N, N + \nu + 1; 1; \frac{1 - \cos 4X}{2}) \\ &= (\cos 2X)^\nu P_N^{(0, \nu)}(\cos 4X) \\ &= d_{\nu/2, \nu/2}^{N/2}(4X). \end{aligned} \quad (5.12)$$

The function $P_n^{(\alpha, \beta)}(x)$ is the Jacobi polynomial of degree n as defined by Magnus, Oberhettinger, and Soni (1966). The function $d_{m, m}^j(\beta)$ is the reduced rotation matrix defined by Rose (1957). The value N appearing in Equation (5.12) must, of course, be a non-negative integer. It is related to the order ℓ of the harmonic by the following relation

$$N = (\ell - \mu)/4 = (\lambda - \nu)/2. \quad (5.13)$$

The λ appearing in Equation (5.13) and in Equation (5.12) is half the value of the order ℓ , which is even. Putting N equal to a non-negative integer is just another way of saying that the order ℓ of the harmonic must be greater than μ by multiples of four. Another way of expressing the same idea is to say that the indices appearing on the rotation matrix of Equation (5.12) must satisfy their usual relations.

Instead of the indices ℓ and μ , the indices λ and ν will be used. The expansion of the wave function given in Equation (5.4) may now be

written

$$\psi(\rho, \chi, \gamma') = \sum_{\lambda=0}^{\infty} \sum_{\substack{\nu=-\lambda \\ \Delta\nu=2}}^{\lambda} \psi_{\lambda\nu}(\rho) d_{\nu/2, \nu/2}^{\lambda/2} (4\chi) \exp(i2\nu\gamma') . \quad (5.14)$$

It is assumed that the potential energy V appearing in Schroedinger's Equation (5.1) is given by a similar expansion, namely:

$$V(\rho, \chi, \gamma') = \sum_{\lambda=0}^{\infty} \sum_{\substack{\nu=-\lambda \\ \Delta\nu=2}}^{\lambda} V_{\lambda\nu}(\rho) d_{\nu/2, \nu/2}^{\lambda/2} (4\chi) \exp(i2\nu\gamma') . \quad (5.15)$$

The expansion for the Coulomb potential is given in Appendix C.

In both Equation (5.15) and Equation (5.14) the expansion coefficients must express the fact that the quantity on the left of the equation is real. Thus, for example, the coefficients $V_{\lambda\nu}(\rho)$ of Equation (5.15) satisfy the relation

$$V_{\lambda\nu}(\rho) = V_{\lambda-\nu}^*(\rho) , \quad (5.16)$$

where the asterisk indicates the complex conjugate. A similar relation holds for the coefficients $\psi_{\lambda\nu}(\rho)$ of Equation (5.14).

Within the computer program the real parts and the imaginary parts of the coefficients must be stored for the following positive values of ν ,

$$\nu = \lambda, \lambda - 2, \lambda - 4, \dots \geq 0 . \quad (5.17)$$

When ν takes the value zero, only the real part of the coefficient needs to be stored, since, according to Equation (5.16), the imaginary part vanishes.

The product $V\psi$ of the potential and the wave function which appears in the Schroedinger Equation (5.1) may also be expanded in a series of harmonics. Application of the Clebsch-Gordan series (Rose 1957) yields the following expression for the coefficients:

$$(V\psi)_{\lambda\nu} = (\lambda + 1) \sum_{\lambda'\nu'} \psi_{\lambda'\nu'}(\rho) M_{\nu'\nu}^{\lambda'\lambda}(\rho), \quad (5.18)$$

where

$$\begin{aligned} M_{\nu'\nu}^{\lambda'\lambda}(\rho) &= (\lambda + 1)^{-1} \sum_{\lambda''\nu''} (c(\lambda'/2 \lambda''/2 \lambda/2; \nu'/2 \nu''/2))^2 v_{\lambda''\nu''}(\rho) \\ &= \sum_{\lambda''\nu''} \frac{(c(\lambda'/2 \lambda/2 \lambda''/2; -\nu'/2 \nu/2))^2}{(\lambda'' + 1)} v_{\lambda''\nu''}(\rho). \end{aligned} \quad (5.19)$$

This last form for M follows from Racah's symmetry relations (Rose 1957) for the Clebsch-Gordan coefficients. It shows that the M's are symmetric, thereby decreasing the storage requirements inside the computer. Specifically, the symmetry relations satisfied by M are

$$M_{\nu\nu'}^{\lambda\lambda'}(\rho) = M_{-\nu'-\nu}^{\lambda'\lambda}(\rho) = (M_{\nu'\nu}^{\lambda'\lambda}(\rho))^*. \quad (5.20)$$

Equation (5.16) has been used in deriving this last symmetry relation in Equation (5.20).

Introducing the coefficients

$$\phi_{\lambda\nu}(\rho) = \rho^{5/2} \psi_{\lambda\nu}(\rho), \quad (5.21)$$

and making the simplest approximation to the second derivative (this simple approximation is made in order to have adequate storage in the fast memory of the computer), namely,

$$\frac{d^2\phi}{d\rho^2}(\rho) = \frac{\phi(\rho + h) + \phi(\rho - h) - 2\phi(\rho)}{h^2}, \quad (5.22)$$

leads to the following difference equation:

$$\phi_{\lambda\nu}(\rho + h) = -\phi_{\lambda\nu}(\rho - h) + (\phi_{\lambda\nu}(\rho) \cdot S_{\lambda}(\rho) + T_{\lambda\nu}(\rho)) c_{\lambda}. \quad (5.23)$$

The quantities appearing in this Equation (5.23) which need defining are

$$S_{\lambda}(\rho) = [((h\rho)^2(2 - 2h^2E) - 0.25h^4)/c_{\lambda} + c_{\lambda}]/(hr)^2, \quad (5.24)$$

$$T_{\lambda\nu}(\rho) = \sum_{\substack{\lambda' \\ \nu'}} M_{\nu'\nu}^{\lambda'\lambda}(\rho) \cdot \phi_{\lambda'\nu'}(\rho), \quad (5.25)$$

and

$$c_{\lambda} = 2h^2(\lambda + 1). \quad (5.26)$$

Planck's constant \hbar is assumed to be unity in these above equations.

The foregoing Equations (5.23) through Equation (5.26) are in a form very suitable for computation purposes, and, in fact, are the equations used in the program. The symmetric array $M_{\nu'\nu}^{\lambda'\lambda}(\rho)$ does not depend on the energy. It is calculated once and for all at the beginning of the program and stored on magnetic tape. As the integration proceeds, it is buffered into the memory of the computer. Of course, this array as well as the terms appearing in both Equation (5.23) and Equation (5.25) must be separated into their real and imaginary parts.

The above describes the method of integrating the Schrodinger equation to obtain the wave function at a given energy. There is still the problem of "guessing" the energy of a bound state. The following

describes the procedure used to consistently improve the estimate of the energy eigenvalue.

The procedure is a direct generalization of that used by Lovitch and Rosati (1965) to integrate the Schroedinger equation for the deuteron. The eigensolution ϕ , consisting of N components, is assumed to satisfy a second-order equation of the form

$$-\frac{d^2\phi}{dr^2} + V(r) \phi = \epsilon\phi, \quad (5.27)$$

along with two-point homogeneous boundary conditions. The operator V is assumed to be a symmetric matrix; ϵ is the eigenvalue desired. The eigensolution ϕ is, of course, continuous and has a continuous derivative everywhere in its domain of definition.

At the "guessed" energy $\epsilon + \delta$, which is not an eigenvalue of the system, the equation

$$-\frac{d^2u}{dr^2} + V(r) u = (\epsilon + \delta) u \quad (5.28)$$

has N independent solutions v which satisfy the inner boundary condition, but no linear combination of these satisfy the outer boundary condition. Similarly, Equation (5.28) also has N independent solutions w which satisfy the outer boundary condition, but, again, no linear combination of these satisfies the inner boundary condition.

By allowing discontinuities in the components of the solutions and their derivatives at an intermediate point a, the match point, one may construct a solution u to Equation (5.28). Thus, the discontinuous solution u is a linear combination of the v's on the left of the match

point and is a linear combination of the w 's on the right of the match point.

From Equation (5.27) and Equation (5.28) the following may be derived:

$$-\phi' \frac{d^2 u}{dr^2} + \frac{d^2 \phi'}{dr^2} u = \delta \phi' u . \quad (5.29)$$

The transpose is again denoted by the prime. Integration of this Equation (5.29) first on the left of the match point and then on the right of the match point yields the following:

$$\delta \int dr \phi' u = \phi'(a) \left[\frac{du}{dr} \right]_a - \frac{d\phi'(a)}{dr} [u]_a , \quad (5.30)$$

where

$$\left[\frac{du}{dr} \right]_a = \frac{du(a+)}{dr} - \frac{du(a-)}{dr} \quad (5.31)$$

is the discontinuity in the derivative of the solution at the match point a , and

$$[u]_a = u(a+) - u(a-) \quad (5.32)$$

is the discontinuity in the solution itself at the match point a .

If two N -dimensional column vectors, α and β , are chosen so that

$$\phi'(a) \cdot \alpha - \frac{d\phi'(a)}{dr} \cdot \beta = 1 , \quad (5.33)$$

and if then the discontinuous solution u is chosen so that its discontinuities at the match point are

$$\left[\frac{du}{dr} \right]_a = k\alpha \quad (5.34)$$

and

$$[u]_a = k\beta \quad (5.35)$$

for some scalar k , then Equation (5.30) for the deviation δ in the eigenvalue becomes

$$\delta \int dr \phi' u = k . \quad (5.36)$$

As yet, there has been made no approximation. However, some approximation to the true eigensolution ϕ must be made in order to calculate the integral appearing on the left of Equation (5.36).

The only reasonable quantity at hand with which to approximate the true solution ϕ is the discontinuous solution u . But there is some liberty in choosing this. A convenient method is to take β to be the null vector and to take α to be the solution $u(a)$ at the match point. In this way the solution u is continuous, only its derivative being discontinuous. The solution u is then chosen so that the discontinuity in the derivative will be as small as possible in some sense.

The assumptions of the foregoing paragraph cause Equation (5.33) to be a normalization condition on u , namely:

$$u'(a) \cdot u(a) = 1 . \quad (5.37)$$

Equation (5.34) becomes under the above assumptions

$$\left[\frac{du}{dr} \right]_a = k u(a) . \quad (5.38)$$

This last equation may be expressed in terms of the complete sets of solutions, v on the left and w on the right. Equation (5.38) becomes

$$\left(\frac{dw}{dr} w^{-1} - \frac{dv}{dr} v^{-1} \right) u = ku . \quad (5.39)$$

All quantities in this Equation (5.39) are evaluated at the match point a . Note that w and v are square matrices, made up from complete sets of solutions, which satisfy the outer and inner boundary conditions, respectively.

The problem of minimizing the discontinuity reduces to that of finding the eigenvalue of Equation (5.39) of minimum modulus. It should be noted that the matrix difference on the left is independent of the particular bases chosen to describe the complete sets of solutions.

The knowledge of the solution $u(a)$ at the match point from the eigensolution belonging to the minimum eigenvalue of Equation (5.39) allows the determination of u over the whole range. The estimate of the energy correction to be made is then given by the following approximation to Equation (5.36):

$$-\delta = -\frac{u'(a)\left[\frac{du}{dr}\right]_a}{\int dr u'u} . \quad (5.40)$$

Equations (5.37) and Equation (5.38) have been used to eliminate k from the expression appearing in Equation (5.40).

Although there seems to be no guarantee that a real minimum exists to the Equation (5.39), intuitively it seems that such a real value should exist. From Equation (5.36) it is seen that such an eigenvalue would correspond to the true solution of the differential system lying nearest to the "guessed" solution. In any case, in practice, the real minimum has always been found to exist.

The results of the calculations of the energy eigenvalues of the helium atom for several values of the order λ of the expansion are given

in Table III. There are two numbers against which these results may be checked. The first number is the zero-order energy value predicted by the formula

$$E_0 = \left(\frac{16}{15\pi}\right)^2 \left[Z_1 Z_2 \sqrt{\frac{2m_1 m_2}{(m_1 + m_2)m_e}} + \dots \right]^2, \quad (5.41)$$

where atomic units have been used. The bracket contains three terms, each of the form shown and differing only by a permutation of the subscripts. This Equation (5.41) follows directly from Equation (70) of the paper by Zickendraht (1965).

Insertion of the masses and charges appropriate to the helium atom into this Equation (5.41) yields for the zero-order energy the value -2.498364151 atomic units. It is seen that the error introduced by the use of a finite mesh and a finite boundary condition is quite small.

The other energy value against which the results given in Table III may be checked is the value -2.9037243 atomic units, obtained from the very accurate calculation by Pekeris (1959). These results shown in Table III should be identical to the energy values given by a variational calculation using the corresponding harmonics as linear variational functions. Note that the calculated energies lie above the "true" value. For the last set of values given in Table III, the computing time required for one iteration was about one hundred seconds. Only three or four iterations are needed. Hence, the results show that the method gives reasonable results for a small amount of calculation time. The complete computer program and a brief set of instructions are given in Appendix D.

TABLE III
HELIUM ATOM ENERGY VALUES FOR VARIOUS ORDERS OF
THE HARMONIC EXPANSION

λ	E (atomic units)
0	-2.498371
1	-2.694048
2	-2.836037

CHAPTER VI

SUMMARY AND DISCUSSION

The purpose of the study reported in this thesis was to develop general methods for the calculation of quantum-mechanical three-body problems. In particular, methods are needed to calculate wave functions of bound systems and scattering systems in which the form of the potential is as general as possible. Previous nonvariational calculations have used restricted forms of the potentials. The variational methods, while giving accurate values for the bound-state energy eigenvalues, are limited to the ground state and a few low-lying excited states. Furthermore, the variational method does not give accurate wave functions.

The method developed herein has been shown to give good results for the bound state of the helium atom. Although this method will not replace the variational method for the calculation of the ground-state energies, it does present a method of calculating wave functions reliably, especially in that region where the three particles are interacting strongly.

Particular systems for which this method appears to be especially useful are the scattering of nucleons by deuterons, direct reactions involving deuterons, and nuclear reactions involving three-body final states.

There are a number of directions in which this study may be continued. An obvious direction is to generalize to systems more complex than the three-body system. The coordinate classification scheme

and the form of the metric tensor are already generalized to an arbitrary number of particles. It should not be difficult to find coordinate systems suitable for an arbitrary number of particles similar to the coordinates developed here for the three- and four-body systems.

Harmonics similar to the ones developed herein for the three-body problem should be developed for these more complex systems. And, again, the reduction of the Schroedinger equation to a set of coupled ordinary differential equations should be possible, allowing a similar numerical integration. Of course, the increased complexity of the harmonic expansion will be a limiting factor.

The continued application to the three-body problem of the methods developed herein may take a number of turns. First, the outer boundary condition of the bound-state problem should be improved. This may be done by using the Wentzel-Kramers-Brillouin approximation at large distances from the origin. Second, the wave function should be given additional degrees of freedom to correspond to spin and I-spin states. Third, realistic nuclear potentials should be used for the development of subroutines which can be inserted into the program for the calculation of the wave functions of the two three-body nuclei ${}^3\text{H}$ and ${}^3\text{He}$. Of course, the computer program itself can be made faster and more efficient.

Perhaps the most advantageous use of the method developed in this thesis would be in its application to collision phenomena. This would require the development of harmonic functions having greater values of the angular momentum than is represented by the S-state functions used

in this thesis. The coupling of these functions with the potential functions would have to be developed also.

In the application to collision phenomena, the wave function should be found by integrating coupled ordinary differential equations over the internal region and matched to an external wave function on some surface where the potential is small. This matching to an external wave function is necessary because the truncated harmonic expansion used in the internal region will not give an adequate representation of the two-body bound states at large distances, as has been pointed out.

The results of the study reported in this thesis indicate that all these goals are feasible ones.

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APPENDICES

APPENDIX A

SURFACE HARMONICS IN N DIMENSIONS

The construction of spherical surface harmonics in N dimensions using the invariantly classified coordinates defined in Chapter II is a difficult problem. A simpler problem is discussed here, namely, that of finding the surface harmonics associated with an orthogonal coordinate system which is a generalization of the ordinary three-dimensional spherical and cylindrical coordinate systems. The classification of surface harmonics in these coordinates is simple because the structure of the subgroups by which the harmonics are classified is obvious. The solution of this simpler problem should help in understanding the structure and classification of N -dimensional spherical harmonics in general as well as being in itself a useful bit of information.

Accordingly, an N -dimensional coordinate system consisting of one radial variable and $N-1$ angular variables will be constructed. The method of construction will proceed by means of orthogonal projections and thence to an orthogonal system of coordinates. These projections, which define the coordinates, may be specified most simply, perhaps, by means of a projection diagram such as that in Figure 4. The line S_0 in the diagram represents the N -dimensional space. Each of the other $N-2$ lines represents a linear subspace of two or more dimensions. The N one-dimensional subspaces are represented by the terminal end points on some of the lines.

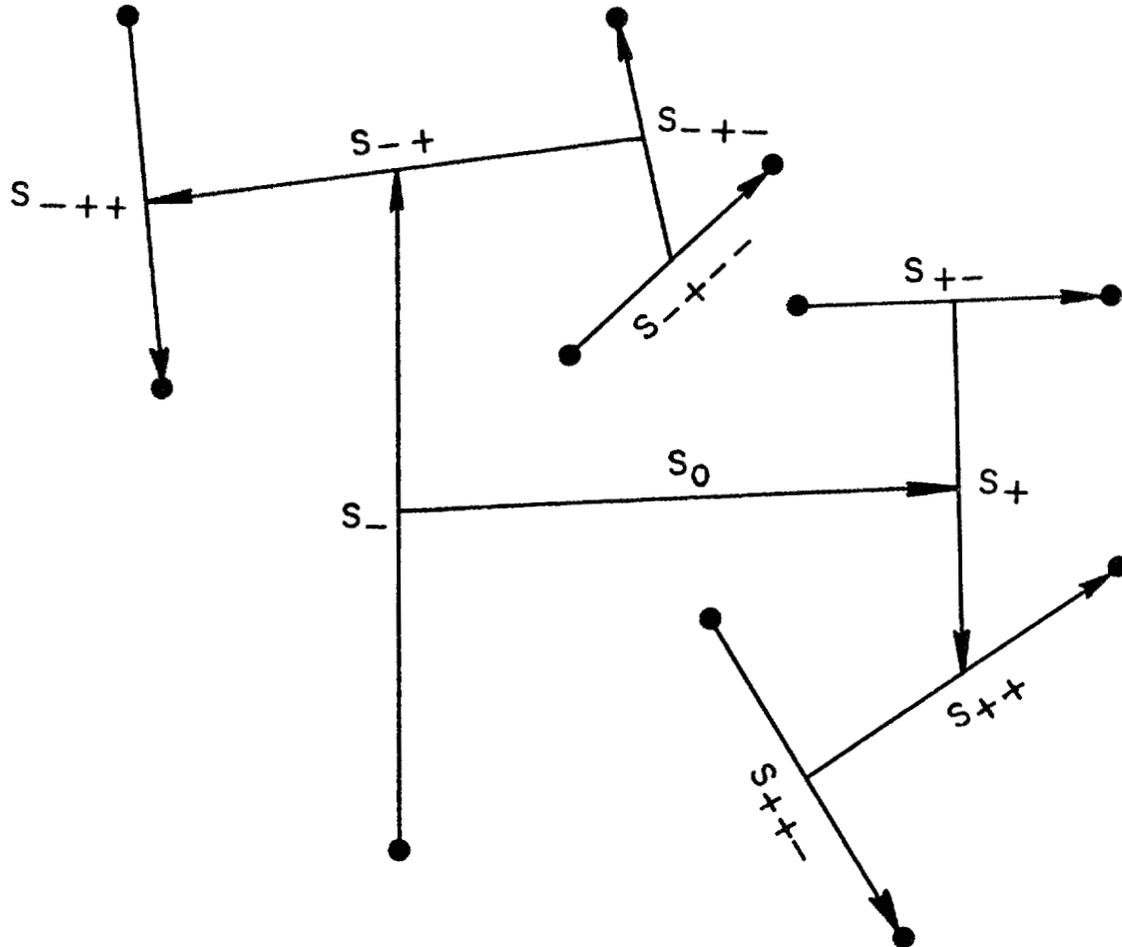


Figure 4. A projection diagram defining angular coordinates in a space of eleven dimensions.

Each subspace of two or more dimensions may be decomposed by means of projections onto two orthogonal subspaces. Thus, each line is terminated by two lines, two points, or a line and a point. An arrow on the line indicates which projection is considered the primary projection and, hence, gets the cosine of the projection angle θ . The secondary projection gets the sine of the projection angle θ .

A vector of length r lying in the space S_0 is projected first onto the subspace S_+ and then onto the orthogonal subspace S_- . The lengths of the projections are $r \cos \theta_0$ and $r \sin \theta_0$, respectively. The primary projection of length $r \cos \theta_0$ lying in subspace S_+ may again be projected onto the subspaces S_{++} and S_{+-} , and so forth, until the vector is decomposed into its one-dimensional rectangular components. The $N-1$ projection angles and the radius r may be taken as orthogonal coordinates.

The range of the variable r is from zero to infinity (if the dimension N is greater than unity). The range of a projection angle is as follows: (1) from zero to 2π if the two subspaces are one-dimensional, (2) from zero to π if only one subspace is one-dimensional, and (3) from zero to $\pi/2$ if neither subspace is one-dimensional.

The element of volume $d\tau$ is given by

$$d\tau = dr \rho_0 d\theta_0 \rho_+ d\theta_+ \rho_- d\theta_- \rho_{++} d\theta_{++} \rho_{+-} d\theta_{+-} \dots, \quad (\text{A.1})$$

where the subscripted notation corresponds with that of the subspace in which the angular displacement is embedded, and ρ_i is the length of the projection of r onto the subspace S_i . An example is

$$\rho_{+++++} = r \cos \theta_0 \sin \theta_+ \sin \theta_{+-} \cos \theta_{+--} \cos \theta_{+---} \cos \theta_{+----} \dots \quad (\text{A.2})$$

The Laplacian operator in this orthogonal system is

$$\nabla^2 = r^{-(N-1)} \frac{\partial}{\partial r} r^{N-1} \frac{\partial}{\partial r} + \dots + \frac{1}{\rho} \frac{\partial}{\partial \theta_i} \frac{\rho}{\rho_i^2} \frac{\partial}{\partial \theta_i} + \dots, \quad (\text{A.3})$$

where ρ is the product of all the ρ_i 's. The subscript i is an abbreviation for a series of +'s and -'s or 0.

Now ρ_j depends on the angle θ_i only if S_j is a subspace of S_i . Looking at the diagram and making the necessary correspondences, one sees that the Laplacian may be written

$$\begin{aligned} \nabla^2 = & r^{-(N-1)} \frac{\partial}{\partial r} r^{N-1} \frac{\partial}{\partial r} + \dots \\ & + \rho_i^{-2} (\cos \theta_i)^{-L_{i+}} (\sin \theta_i)^{-L_{i-}} \frac{\partial}{\partial \theta_i} (\cos \theta_i)^{L_{i+}} (\sin \theta_i)^{L_{i-}} \frac{\partial}{\partial \theta_i} + \dots, \end{aligned} \quad (\text{A.4})$$

where L_{i+} is the number of lines on the primary side of the line S_i and L_{i-} is the number of lines on the secondary side. The number L_i is associated with the dimension N_i of the subspace S_i by the relation

$$N_i = L_i + 1. \quad (\text{A.5})$$

Obviously,

$$L_i = L_{i+} + L_{i-} + 1. \quad (\text{A.6})$$

The terms of Equation (A.4) may be arranged to give the form

$$\begin{aligned} \nabla^2 = & \frac{1}{r^{N-1}} \frac{\partial}{\partial r} r^{N-1} \frac{\partial}{\partial r} \\ & + \frac{1}{r^2} \left\{ \frac{1}{(\cos \theta_o)^{L_+} (\sin \theta_o)^{L_-}} \frac{\partial}{\partial \theta_o} (\cos \theta_o)^{L_+} (\sin \theta_o)^{L_-} \frac{\partial}{\partial \theta_o} \right. \end{aligned}$$

continued

$$\begin{aligned}
& + \frac{1}{\cos^2 \theta_+} \left[\frac{1}{(\cos \theta_+)^{L_{++}} (\sin \theta_+)^{L_{+-}}} \frac{\partial}{\partial \theta_+} (\cos \theta_+)^{L_{++}} (\sin \theta_+)^{L_{+-}} \frac{\partial}{\partial \theta_+} \right. \\
& \quad \left. + \frac{1}{\cos^2 \theta_+} (\dots) + \frac{1}{\sin^2 \theta_+} (\dots) \right] \\
& + \frac{1}{\sin^2 \theta_-} \left[\frac{1}{(\cos \theta_-)^{L_{-+}} (\sin \theta_-)^{L_{--}}} \frac{\partial}{\partial \theta_-} (\cos \theta_-)^{L_{-+}} (\sin \theta_-)^{L_{--}} \frac{\partial}{\partial \theta_-} \right. \\
& \quad \left. + \frac{1}{\cos^2 \theta_-} (\dots) + \frac{1}{\sin^2 \theta_-} (\dots) \right] \Big\} . \tag{A.7}
\end{aligned}$$

Solutions of Laplace's equation

$$\nabla^2 Y = 0 \tag{A.8}$$

may be found easily since the equation is separable. The solution is of the form

$$Y = f(r) y_0 y_+ y_- y_{++} y_{+-} y_{-+} y_{--} y_{+++} \dots , \tag{A.9}$$

where each y_i satisfies an equation of the form

$$\left\{ \frac{1}{(\cos \theta_i)^{L_{i+}} (\sin \theta_i)^{L_{i-}}} \frac{d}{d\theta_i} (\cos \theta_i)^{L_{i+}} (\sin \theta_i)^{L_{i-}} \frac{d}{d\theta_i} \right. \\
\left. - \frac{M_{i+}}{\cos^2 \theta_i} - \frac{M_{i-}}{\sin^2 \theta_i} - M_i \right\} y_i = 0 . \tag{A.10}$$

The M_i 's are separation constants.

A change from the dependent variable y_i to the dependent variable u_i defined by

$$u_i = (\cos \theta_i)^{\frac{1}{2}L_{i+}} (\sin \theta_i)^{\frac{1}{2}L_{i-}} y_i \quad (\text{A.11})$$

transforms Equation (A.10) into the following:

$$\frac{d^2 u_i}{d\theta_i^2} + \left[\frac{1 - 4\alpha_i^2}{4 \sin^2 \theta_i} + \frac{1 - 4\beta_i^2}{4 \cos^2 \theta_i} + (2n_i + \alpha_i + \beta_i + 1)^2 \right] u_i = 0. \quad (\text{A.12})$$

The parameters α_i and β_i are defined by

$$1 - 4\alpha_i^2 = -4M_{i-} + L_{i-}(2 - L_{i-}) \quad (\text{A.13})$$

and

$$1 - 4\beta_i^2 = -4M_{i+} + L_{i+}(2 - L_{i+}). \quad (\text{A.14})$$

The parameter n_i is related to M_i according to

$$M_i + \frac{(L_i - 1)^2}{4} = (2n_i + \alpha_i + \beta_i + 1)^2. \quad (\text{A.15})$$

The harmonic functions y_i must be regular for all values of the projection angle θ_i which have physical meaning. They must also form polynomials in the rectangular components of the N-dimensional vector. Either of these requirements leads to nonnegative integral values for the n_i 's of Equation (A.12). The solutions u_i are given in terms of Jacobi polynomials (Magnus, Oberhettinger, and Soni 1966) as follows:

$$u_i = (\sin \theta_i)^{\alpha_i + \frac{1}{2}} (\cos \theta_i)^{\beta_i + \frac{1}{2}} P_{n_i}^{(\alpha_i, \beta_i)}(\cos 2\theta_i). \quad (\text{A.16})$$

The corresponding solutions for the y_i 's are

$$y_i = (\sin \theta_i)^{\alpha_i - \frac{1}{2}(L_{i-} - 1)} (\cos \theta_i)^{\beta_i - \frac{1}{2}(L_{i+} - 1)} P_{n_i}^{(\alpha_i, \beta_i)}(\cos 2\theta_i). \quad (\text{A.17})$$

In a subspace S_i of dimension N_i there exist surface harmonics of the form

$$Y_i = y_i y_{i+} y_{i-} y_{-++} y_{i+-} \dots \quad (\text{A.18})$$

The order ℓ_i of these surface harmonics is the degree of the corresponding polynomial in the components of an N_i -dimensional vector. The order ℓ_i is related to the separation constant M_i by the following equation:

$$M_i = \ell_i (\ell_i + N_i - 2) . \quad (\text{A.19})$$

Substituting into this the relations of Equation (A.5) and Equation (A.15) results in the following:

$$\ell_i = 2n_i + \alpha_i + \beta_i + \frac{1}{2}(3 - L_i) \geq 0 . \quad (\text{A.20})$$

The combination of Equation (A.13), Equation (A.15), and the inequality on the right of Equation (A.20) leads to the following condition on α_i :

$$\alpha_i = 2n_{i-} + 1 + \alpha_{i-} + \beta_{i-} \geq \frac{1}{2}(L_{i-} - 1) . \quad (\text{A.21})$$

A similar condition on β_i is

$$\beta_i = 2n_{i+} + 1 + \alpha_{i+} + \beta_{i+} \geq \frac{1}{2}(L_{i+} - 1) . \quad (\text{A.22})$$

It is thus seen that α_i is an even or odd multiple of one-half according as L_{i-} is odd or even. For the particular case that L_{i-} vanishes, α_i may take on either of the two values: $+\frac{1}{2}$, $-\frac{1}{2}$. For all other values of L_{i-} the value of α_i is uniquely determined by Equation (A.21). Corresponding statements apply for β_i and its relation to L_{i+} .

Thus, the spherical surface harmonics in N dimensions may be characterized by N signs (± 1) , one sign for each rectangular dimension, and $N-1$ nonnegative integers n_i , one associated with each projection angle. The order ℓ_0 of the harmonic is

$$\ell = 2 \sum_{n_i} + \frac{1}{2}N + \frac{1}{2} \sum (\pm 1) , \quad (\text{A.23})$$

wherein the summation over the n_i 's has $N-1$ terms, one for each projection angle θ_i , and the second summation over the signs has N terms, one for each one-dimensional linear subspace.

The number of harmonics of order ℓ in a space of N dimensions may be found by summing over all the possible ways in which Equation (A.23) may be satisfied. The result is

$$\sum_r \frac{(r + N - 2)! N(N - 1)}{r!(\ell - 2r)! (N - \ell + 2r)!} . \quad (\text{A.24})$$

APPENDIX B

DETAILS OF THE METRIC TENSOR

In this appendix the metric tensor and related quantities, as discussed in Chapter III, are considered in detail. Results for the special cases of the two-, three-, and four-body systems are each presented separately. Some general results for N particles are also explicitly given.

The nomenclature and symbols are the same as in Chapter III.

The Two-Body System

The metric tensor for the two-body system is well known. The results are given here for completeness and for illustration of the application of the method to a simple system.

The size coordinate frequently chosen is the interparticle distance r_{12} , which is related to the radius of gyration ρ through the following:

$$r_{12} = \left(\frac{m}{\mu}\right)^{\frac{1}{2}} \rho, \quad (\text{B.1})$$

where the total mass is

$$m = m_1 + m_2, \quad (\text{B.2})$$

and the reduced mass is

$$\mu = \frac{m_1 m_2}{m_1 + m_2}. \quad (\text{B.3})$$

The rotational coordinates frequently chosen are the polar angle θ and

the azimuthal angle ϕ , which are related to the Euler angles α and β by the relations:

$$\theta = \beta \quad (\text{B.4})$$

and

$$\phi = \alpha - \pi/2 . \quad (\text{B.5})$$

Because of the simplicity of the two-body problem, some of the rows and columns of the matrices vanish. These are omitted. The coordinate matrix r in the observer's reference frame takes the form

$$r = m^{\frac{1}{2}} \begin{bmatrix} \sin \beta \cos(\alpha - \frac{\pi}{2}) & X \\ \cos \beta \sin(\alpha - \frac{\pi}{2}) & Y \\ \cos \beta & Z \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \rho \\ 0 \\ 0 \\ 1 \end{bmatrix} \begin{bmatrix} \sqrt{\frac{m_2}{m_1+m_2}} - \sqrt{\frac{m_1}{m_1+m_2}} \\ \sqrt{\frac{m_1}{m_1+m_2}} \\ \sqrt{\frac{m_2}{m_1+m_2}} \end{bmatrix} \times \begin{bmatrix} m_1^{-\frac{1}{2}} & 0 \\ 0 & m_2^{-\frac{1}{2}} \end{bmatrix} . \quad (\text{B.6})$$

Although only one column of the rotation matrix appears in Eq. (B.6), the complete matrix is needed to get all three components of the angular velocity ω . The third Euler angle, which is not needed in the two-body problem, does not appear. The matrix is

$$R = \begin{bmatrix} \cos \alpha & -\cos \beta \sin \alpha & \sin \beta \sin \alpha \\ \sin \alpha & \cos \beta \cos \alpha & -\sin \beta \cos \alpha \\ 0 & \sin \beta & \cos \beta \end{bmatrix} . \quad (\text{B.7})$$

The corresponding time derivative is given in terms of the elements of the rotation matrix itself by

$$\dot{R} = \begin{bmatrix} -R_{21} & -R_{22} & -R_{23} \\ R_{11} & R_{12} & R_{13} \\ 0 & 0 & 0 \end{bmatrix} \dot{\alpha} + \begin{bmatrix} 0 & R_{13} & -R_{12} \\ 0 & R_{23} & -R_{22} \\ 0 & R_{33} & -R_{32} \end{bmatrix} \dot{\beta} . \quad (\text{B.8})$$

The angular velocities are then found from

$$\dot{R}'R = \begin{bmatrix} 0 & R_{33} & -R_{32} \\ -R_{33} & 0 & R_{31} \\ R_{32} & -R_{31} & 0 \end{bmatrix} \dot{\alpha} + \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix} \dot{\beta} \quad (\text{B.9})$$

by using the values of the elements of the rotation matrix given in Equation (B.7). The angular velocity in the body system is accordingly

$$\omega = \begin{bmatrix} 0 \\ \sin \beta \\ \cos \beta \end{bmatrix} \dot{\alpha} + \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \dot{\beta} = \begin{bmatrix} 0 & 1 \\ \sin \beta & 0 \\ \cos \beta & 0 \end{bmatrix} \begin{bmatrix} \dot{\alpha} \\ \dot{\beta} \end{bmatrix} . \quad (\text{B.10})$$

Since one axis is associated with a vanishing moment of inertia, only two components of the angular velocity appear in the kinetic energy. The corresponding truncated matrix for $\bar{\omega}$ is

$$\bar{\omega} = \begin{bmatrix} 0 & 1 \\ \sin \beta & 0 \end{bmatrix} . \quad (\text{B.11})$$

Only one plane moment of inertia does not vanish, namely:

$$\Lambda_3 = m\rho^2 = \mu r_{12}^2 . \quad (\text{B.12})$$

The matrix J containing the ordinary moments of inertia is

$$J = m\rho^2 \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} . \quad (\text{B.13})$$

There are no internal coordinates in the two-body problem. Accordingly the matrix E, the elements of which vanish anyway, is not required in the formation of the metric tensor.

Assuming that the translational coordinates are the rectangular components of the center of mass, X, Y, and Z, that the size coordinate is r_{12} , and that the rotational coordinates are θ and ϕ , the matrices \mathcal{M} and S which form the metric tensor are

$$\mathcal{M} = M \begin{bmatrix} 1 & & & & & \\ & 1 & & & & \\ & & 1 & & & \\ & & & 1 & & \\ & & & & \rho^2 & \\ & & & & & \rho^2 \end{bmatrix} \quad (\text{B.14})$$

and

$$S = \begin{bmatrix} 1 & & & & & \\ & 1 & & & & \\ & & 1 & & & \\ & & & \sqrt{1/m} & & \\ & & & & 0 & 1 \\ & & & & \sin \theta & 0 \end{bmatrix} , \quad (\text{B.15})$$

respectively.

The metric tensor itself is found to be the following well known diagonal expression:

$$J = \begin{bmatrix} \Lambda_2 & & \\ & \Lambda_1 & \\ & & \Lambda_1 + \Lambda_2 \end{bmatrix} = \begin{bmatrix} \rho_2^2 & & \\ & \rho_1^2 & \\ & & \rho_1^2 + \rho_2^2 \end{bmatrix} = \rho^2 \begin{bmatrix} \sin^2 \chi & & \\ & \cos^2 \chi & \\ & & 1 \end{bmatrix}. \quad (\text{B.19})$$

The related matrix E has only one component which does not vanish, namely:

$$E_{33} = \sqrt{4\Lambda_1\Lambda_2} = 2\rho_1\rho_2 = \rho^2 \sin 2\chi. \quad (\text{B.20})$$

The matrix $\partial\rho$ of partial derivatives appearing in S is

$$\partial\rho = \begin{bmatrix} \cos \chi & -\rho \sin \chi \\ \sin \chi & \rho \cos \chi \end{bmatrix}. \quad (\text{B.21})$$

The corresponding inverse is

$$(\partial\rho)^{-1} = \begin{bmatrix} \cos \chi & \sin \chi \\ \frac{-\sin \chi}{\rho} & \frac{\cos \chi}{\rho} \end{bmatrix}. \quad (\text{B.22})$$

The internal coordinate γ' describes the internal motion through the matrix

$${}^0_{t'} = \begin{bmatrix} \cos \gamma' & -\sin \gamma' \\ \sin \gamma' & \cos \gamma' \end{bmatrix}. \quad (\text{B.23})$$

The time derivative of this is

$$\dot{{}^0_{t'}} = \begin{bmatrix} -\sin \gamma' & -\cos \gamma' \\ \cos \gamma' & -\sin \gamma' \end{bmatrix} \dot{\gamma}'. \quad (\text{B.24})$$

It follows that

$$\ddot{0}_{t'} \dot{0}'_{t'} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \dot{\gamma}' . \quad (\text{B.25})$$

The single component of u which enters into the kinetic energy is accordingly

$$u = \dot{\gamma}' , \quad (\text{B.26})$$

and the corresponding \bar{u} appearing in S is

$$\bar{u} = 1 . \quad (\text{B.27})$$

The choice of a graph for the three-body system must be made.

There are three such graphs. The one chosen is that appearing in Figure 1, page 20, which has a corresponding matrix

$$O_m = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \sqrt{m_3} & -\sqrt{m_1+m_2} \\ 0 & \sqrt{m_1+m_2} & \sqrt{m_3} \end{bmatrix} \begin{bmatrix} \sqrt{\frac{m_2}{m_1+m_2}} & -\sqrt{\frac{m_1}{m_1+m_2}} & 0 \\ \sqrt{\frac{m_1}{m_1+m_2}} & \sqrt{\frac{m_2}{m_1+m_2}} & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$= \begin{bmatrix} \sqrt{\frac{m_2}{m_1+m_2}} & -\sqrt{\frac{m_1}{m_1+m_2}} & 0 \\ \sqrt{\frac{m_1 m_3}{m_1+m_2}} & \sqrt{\frac{m_2 m_3}{m_1+m_2}} & -\sqrt{m_1+m_2} \\ \sqrt{m_1} & \sqrt{m_2} & \sqrt{m_3} \end{bmatrix} . \quad (\text{B.28})$$

$$g_2 = \begin{bmatrix} \frac{1}{2} \sin^2 \beta (1 + \cos 2\chi \cos 2\gamma) & -\frac{1}{2} \sin \beta \sin 2\chi \sin 2\gamma & \cos \gamma & \sin 2\chi \cos \gamma \\ -\frac{1}{2} \sin \beta \sin 2\chi \sin 2\gamma & \frac{1}{2} (1 - \cos 2\chi \cos 2\gamma) & 0 & 0 \\ \cos \gamma & 0 & 1 & \sin 2\chi \\ \sin 2\chi \cos \gamma & 0 & \sin 2\chi & 1 \end{bmatrix} .$$

(B.34)

The corresponding determinants are

$$|m| = (1/16) \rho^8 \sin^2 4\chi , \quad (B.35)$$

$$|S| = -\rho \sin \beta , \quad (B.36)$$

and

$$|g_{ij}| = (1/16) \rho^{10} \sin^2 4\chi \sin^2 \beta . \quad (B.37)$$

The contravariant components of the metric are given by the inverse of the metric tensor above. For this the following matrices are useful:

$$\bar{J} = \begin{bmatrix} \frac{1}{\Lambda_2} & & & \\ & \frac{1}{\Lambda_1} & & \\ & & \frac{\Lambda_1 + \Lambda_2}{(\Lambda_1 - \Lambda_2)^2} & \\ & & & \frac{1}{(\rho_1^2 - \rho_2^2)^2} \end{bmatrix} = \begin{bmatrix} \frac{1}{\rho_2^2} & & & \\ & \frac{1}{\rho_1^2} & & \\ & & & \frac{1}{(\rho_1^2 - \rho_2^2)^2} \end{bmatrix}$$

$$= \rho^{-2} \begin{bmatrix} \csc^2 \chi & & & \\ & \sec^2 \chi & & \\ & & & \sec^2 2\chi \end{bmatrix} , \quad (B.38)$$

The inverse of the metric tensor decomposes as follows:

$$(g_{ij})^{-1} = \begin{bmatrix} g_1^{-1} & \\ & \rho^{-2} g_2^{-1} \end{bmatrix}, \quad (\text{B.42})$$

where g_1^{-1} is given by

$$g_1^{-1} = \begin{bmatrix} 1 & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & 1 & \\ & & & & \rho^{-2} \end{bmatrix}, \quad (\text{B.43})$$

and g_2^{-1} is given by

$$g_2^{-1} = \begin{bmatrix} G_{11} & G_{21} & -G_{11} \cos \beta & 0 \\ G_{21} & G_{22} & -G_{21} \cos \beta & 0 \\ -G_{11} \cos \beta & -G_{21} \cos \beta & G_{11} \cos^2 \beta + \sec^{-2} 2X & -\sin 2X \sec^2 2X \\ 0 & 0 & -\sin 2X \sec^2 2X & \sec^2 2X \end{bmatrix}. \quad (\text{B.44})$$

The as yet undefined matrix elements appearing in the above symmetric matrix g_2^{-1} are given by:

$$G_{11} = 2(1 - \cos 2X \cos 2\gamma) \csc^2 \beta \csc^2 2X, \quad (\text{B.45})$$

$$G_{21} = 2 \sin 2\gamma \cos 2X \csc \beta \csc^2 2X, \quad (\text{B.46})$$

and

$$G_{22} = 2(1 + \cos 2X \cos 2\gamma) \csc^2 2X. \quad (\text{B.47})$$

The order of the variables has been assumed throughout to be $X, Y, Z, \rho, \chi, \alpha, \beta, \gamma,$ and γ' .

The Four-Body System

The four-body system is the simplest system for which all three moments are nonvanishing. Hence, all three columns of the rotation matrix are needed.

There are three internal coordinates which must describe the three-by-three orthogonal matrix O_t . These internal coordinates may be chosen in analogy to the Euler angles which appear in the rotation matrix R .

In fact, if $R(\alpha, \beta, \gamma)$ is the rotation matrix as a function of the Euler angles α , β , and γ , then the matrix O_t may be defined by

$$O_t = R'(\alpha', \beta', \gamma'). \quad (\text{B.48})$$

This, together with the following definition of O_m in Equation (B.52), may be taken as the definition of the internal coordinates, α' , β' , and γ' .

Equation (B.56) may be used to calculate the internal angular velocities which are given by

$$u_{ij} = (\dot{O}_t, O_t')_{ij} = (\dot{R}'R)_{ij} = - (R'\dot{R})_{ij}. \quad (\text{B.49})$$

Substituting the internal coordinates α' , β' , and γ' for the Euler angles results in

$$u = \bar{u} \begin{bmatrix} \dot{\alpha}' \\ \dot{\beta}' \\ \dot{\gamma}' \end{bmatrix}, \quad (\text{B.50})$$

where \bar{u} is the matrix

$$\bar{u} = \begin{bmatrix} -\sin \beta' \sin \gamma' & -\cos \gamma' & 0 \\ -\sin \beta' \cos \gamma' & \sin \gamma' & 0 \\ -\cos \beta' & 0 & -1 \end{bmatrix}. \quad (\text{B.51})$$

There are fifteen four-body graphs. The graph shown in Figure 1, page 20, corresponds to the matrix

$$O_m = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \sqrt{m_3+m_4} & 0 & -\sqrt{m_1+m_2} \\ 0 & 0 & 1 & 0 \\ 0 & \sqrt{m_1+m_2} & 0 & \sqrt{m_3+m_4} \end{bmatrix}$$

$$\times \begin{bmatrix} \sqrt{\frac{m_2}{m_1+m_2}} & -\sqrt{\frac{m_1}{m_1+m_2}} & 0 & 0 \\ \sqrt{\frac{m_1}{m_1+m_2}} & \sqrt{\frac{m_2}{m_1+m_2}} & 0 & 0 \\ 0 & 0 & \sqrt{\frac{m_4}{m_3+m_4}} & -\sqrt{\frac{m_3}{m_3+m_4}} \\ 0 & 0 & \sqrt{\frac{m_3}{m_3+m_4}} & \sqrt{\frac{m_4}{m_3+m_4}} \end{bmatrix}$$

continued.....

$$= \begin{bmatrix} \sqrt{\frac{m_2}{m_1+m_2}} & -\sqrt{\frac{m_1}{m_1+m_2}} & 0 & 0 \\ \sqrt{\frac{(m_3+m_4)m_1}{m_1+m_2}} & \sqrt{\frac{(m_3+m_4)m_2}{m_1+m_2}} & -\sqrt{\frac{(m_1+m_2)m_3}{m_3+m_4}} & -\sqrt{\frac{(m_1+m_2)m_4}{m_3+m_4}} \\ 0 & 0 & \sqrt{\frac{m_4}{m_3+m_4}} & -\sqrt{\frac{m_3}{m_3+m_4}} \\ \sqrt{m_1} & \sqrt{m_2} & \sqrt{m_3} & \sqrt{m_4} \end{bmatrix} \quad (\text{B.52})$$

It has been assumed that the total mass of the system is unity.

All the quantities required to calculate the coordinate matrix of Equation (2.29) for the four-body system are thus provided above or in a following section containing general results.

For the four-body metric tensor, the general result of Equation (B.73) may be used to give the submatrix $u'Ju$ as well as $\bar{\omega}'J\bar{\omega}$ simply by replacing the Euler angles α , β , and γ , by the internal angles α' , β' , and γ' .

The submatrix $\bar{\omega}'J\bar{u}$ for the four-body system is the sum of three terms:

$$\bar{\omega}'J\bar{u} = M\rho^2 \sin 2\eta \sin \chi \begin{bmatrix} \sin \beta \sin \gamma \sin \beta' \sin \gamma' & \sin \beta \sin \gamma \cos \gamma' & 0 \\ \cos \gamma \sin \beta' \sin \gamma' & \cos \gamma \cos \gamma' & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

continued.....

$$\begin{aligned}
& + M_0^2 \sin 2\eta \cos \chi \begin{bmatrix} \sin \beta \cos \gamma \sin \beta' \cos \gamma' & -\sin \beta \cos \gamma \sin \gamma' & 0 \\ -\sin \gamma \sin \beta' \cos \gamma' & \sin \gamma \sin \gamma' & 0 \\ 0 & 0 & 0 \end{bmatrix} \\
& + M_0^2 \sin^2 \eta \sin 2\chi \begin{bmatrix} \cos \beta \cos \beta' & 0 & \cos \beta \\ 0 & 0 & 0 \\ \cos \beta' & 0 & 1 \end{bmatrix}. \quad (\text{B.53})
\end{aligned}$$

The Rotation Matrix

The rotation matrix is given in terms of the Euler angles (the line of nodes is measured off through the angle α from the x-axis in a right-handed system (Goldstein 1953)) by the following:

R =

$$\begin{bmatrix} \cos \gamma \cdot \cos \alpha - \sin \gamma \cdot \cos \beta \sin \alpha & -\sin \gamma \cdot \cos \alpha - \cos \gamma \cdot \cos \beta \cdot \sin \alpha & \sin \beta \cdot \sin \alpha \\ \cos \gamma \cdot \sin \alpha + \sin \gamma \cdot \cos \beta \cos \alpha & -\sin \gamma \cdot \sin \alpha + \cos \gamma \cdot \cos \beta \cdot \cos \alpha & -\sin \beta \cdot \cos \alpha \\ \sin \gamma \cdot \sin \beta & \cos \gamma \cdot \sin \beta & \cos \beta \end{bmatrix}. \quad (\text{B.54})$$

The columns of R are the observer's coordinates for the unit basis vectors along the principal axes.

The time derivative of R is given by three matrix terms in the following manner:

$$\dot{R} = \begin{bmatrix} -R_{21} & -R_{22} & -R_{23} \\ R_{11} & R_{12} & R_{13} \\ 0 & 0 & 0 \end{bmatrix} \dot{\alpha} + \begin{bmatrix} R_{13} \sin \gamma & R_{13} \cos \gamma & -R_{11} \sin \gamma & -R_{12} \cos \gamma \\ -R_{23} \sin \gamma & R_{23} \cos \gamma & -R_{21} \sin \gamma & -R_{22} \cos \gamma \\ R_{33} \sin \gamma & R_{33} \cos \gamma & -R_{31} \sin \gamma & -R_{32} \cos \gamma \end{bmatrix} \dot{\beta} \\ + \begin{bmatrix} R_{12} & -R_{11} & 0 \\ R_{22} & -R_{21} & 0 \\ R_{32} & -R_{31} & 0 \end{bmatrix} \dot{\gamma} . \quad (\text{B.55})$$

The corresponding result for the matrix product $R' \dot{R}$, which gives the components of the angular velocity in the body system, is

$$R' \dot{R} = \begin{bmatrix} 0 & -\cos \beta & \sin \beta \cos \gamma \\ \cos \beta & 0 & -\sin \beta \sin \gamma \\ -\sin \beta \cos \gamma & \sin \beta \sin \gamma & 0 \end{bmatrix} \dot{\alpha} \\ + \begin{bmatrix} 0 & 0 & -\sin \gamma \\ 0 & 0 & -\cos \gamma \\ \sin \gamma & \cos \gamma & 0 \end{bmatrix} \dot{\beta} + \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \dot{\gamma} . \quad (\text{B.56})$$

The angular velocities in the body system are then given by ω in the form

$$\omega = \bar{\omega} \begin{bmatrix} \dot{\alpha} \\ \dot{\beta} \\ \dot{\gamma} \end{bmatrix} , \quad (\text{B.57})$$

where $\bar{\omega}$ is the matrix appearing in the matrix S and is given by

$$\bar{\omega} = \begin{bmatrix} \sin \beta \sin \gamma & \cos \gamma & 0 \\ \sin \beta \cos \gamma & -\sin \gamma & 0 \\ \cos \beta & 0 & 1 \end{bmatrix}. \quad (\text{B.58})$$

Associated with this matrix $\bar{\omega}$ are its determinant

$$|\bar{\omega}| = -\sin \beta, \quad (\text{B.59})$$

and its inverse

$$\bar{\omega}^{-1} = \begin{bmatrix} \sin \gamma \csc \beta & \cos \gamma \csc \beta & 0 \\ \cos \gamma & -\sin \gamma & 0 \\ -\sin \gamma \cot \beta & -\cos \gamma \cot \beta & 1 \end{bmatrix}. \quad (\text{B.60})$$

The Size Coordinates

A spherical coordinate system is useful for specifying the ρ_1 , ρ_2 , and the ρ_3 of Equation (2.27). The spherical coordinates may be defined by the following:

$$\rho_1 = \rho \sin \eta \cos \chi, \quad (\text{B.61})$$

$$\rho_2 = \rho \sin \eta \sin \chi, \quad (\text{B.62})$$

and

$$\rho_3 = \rho \cos \eta. \quad (\text{B.63})$$

The corresponding matrix $(\partial\rho)$, which appears in S, is

$$(\partial\rho) = \begin{bmatrix} \sin \eta \cos \chi & \rho \cos \eta \cos \chi & -\rho \sin \eta \sin \chi \\ \sin \eta \sin \chi & \rho \cos \eta \sin \chi & \rho \sin \eta \cos \chi \\ \cos \eta & -\rho \sin \eta & 0 \end{bmatrix}, \quad (\text{B.64})$$

and the inverse is

$$(\partial\rho)^{-1} = \begin{bmatrix} \sin \eta \cos \chi & \sin \eta \sin \chi & \cos \eta \\ \frac{\cos \eta \cos \chi}{\rho} & \frac{\cos \eta \sin \chi}{\rho} & \frac{-\sin \eta}{\rho} \\ \frac{-\sin \chi}{\rho \sin \eta} & \frac{\cos \chi}{\rho \sin \eta} & 0 \end{bmatrix}. \quad (\text{B.65})$$

The following appears in the metric tensor:

$$(\partial\rho)'(\partial\rho) = \begin{bmatrix} 1 & & \\ & \rho^2 & \\ & & \rho^2 \sin^2 \eta \end{bmatrix}. \quad (\text{B.66})$$

Appearing in a similar way in the reciprocal of the metric tensor is

$$(\partial\rho)^{-1}(\partial\rho)' = \begin{bmatrix} 1 & & \\ & \rho^{-2} & \\ & & (\rho \sin \eta)^{-2} \end{bmatrix}. \quad (\text{B.67})$$

The forms of the matrices J , E , \bar{J} , and \bar{E} in the various size coordinates are given herewith:

$$J = \begin{bmatrix} (\Lambda_2 + \Lambda_3) & & \\ & (\Lambda_3 + \Lambda_1) & \\ & & (\Lambda_1 + \Lambda_2) \end{bmatrix}$$

$$= M \begin{bmatrix} (\rho_2^2 + \rho_3^2) & & \\ & (\rho_3^2 + \rho_1^2) & \\ & & (\rho_1^2 + \rho_2^2) \end{bmatrix}$$

continued.....

$$= M\rho^2 \begin{bmatrix} 1 - \sin^2\eta \cos^2\chi & & \\ & 1 - \sin^2\eta \sin^2\chi & \\ & & 1 - \cos^2\eta \end{bmatrix}, \quad (\text{B.68})$$

$$E = \begin{bmatrix} \sqrt{4\Lambda_2\Lambda_3} & & \\ & \sqrt{4\Lambda_3\Lambda_1} & \\ & & \sqrt{4\Lambda_1\Lambda_2} \end{bmatrix} = 2M \begin{bmatrix} \rho_2\rho_3 & & \\ & \rho_3\rho_1 & \\ & & \rho_1\rho_2 \end{bmatrix}$$

$$= M\rho^2 \begin{bmatrix} \sin 2\eta \sin \chi & & \\ & \sin 2\eta \cos \chi & \\ & & \sin^2\eta \sin 2\chi \end{bmatrix}, \quad (\text{B.69})$$

$$\bar{J} = \begin{bmatrix} \frac{\Lambda_2 + \Lambda_3}{(\Lambda_2 - \Lambda_3)^2} & & \\ & \frac{\Lambda_3 + \Lambda_1}{(\Lambda_3 - \Lambda_1)^2} & \\ & & \frac{\Lambda_1 + \Lambda_2}{(\Lambda_1 - \Lambda_2)^2} \end{bmatrix}$$

$$= \frac{1}{M} \begin{bmatrix} \frac{\rho_2^2 + \rho_3^2}{(\rho_2^2 - \rho_3^2)^2} & & \\ & \frac{\rho_3^2 + \rho_1^2}{(\rho_3^2 - \rho_1^2)^2} & \\ & & \frac{\rho_1^2 + \rho_2^2}{(\rho_1^2 - \rho_2^2)^2} \end{bmatrix}$$

continued.....

$$= \frac{1}{M\rho^2} \left[\begin{array}{c} \frac{(1 - \sin^2\eta \cos^2\chi)}{(\cos 2\eta + \sin^2\eta \cos^2\chi)^2} \\ \frac{(1 - \sin^2\eta \sin^2\chi)}{(\cos 2\eta + \sin^2\eta \sin^2\chi)^2} \\ \frac{1}{\cos^2 2\chi \sin^2\eta} \end{array} \right],$$

(B.70)

$$\bar{E} = \left[\begin{array}{c} \frac{\sqrt{4\Lambda_2\Lambda_3}}{(\Lambda_2 - \Lambda_3)^2} \\ \frac{\sqrt{4\Lambda_3\Lambda_1}}{(\Lambda_3 - \Lambda_1)^2} \\ \frac{\sqrt{4\Lambda_1\Lambda_2}}{(\Lambda_1 - \Lambda_2)^2} \end{array} \right]$$

$$= \frac{1}{M} \left[\begin{array}{c} \frac{2\rho_2\rho_3}{(\rho_2^2 - \rho_3^2)^2} \\ \frac{2\rho_3\rho_1}{(\rho_3^2 - \rho_1^2)^2} \\ \frac{2\rho_1\rho_2}{(\rho_1^2 - \rho_2^2)^2} \end{array} \right]$$

continued.....

$$= \frac{1}{M_0^2} \begin{bmatrix} \frac{\sin 2\eta \sin \chi}{(\cos 2\eta + \sin^2\eta \cos^2\chi)^2} & & \\ & \frac{\sin 2\eta \cos \chi}{(\cos 2\eta + \sin^2\eta \sin^2\chi)^2} & \\ & & \frac{\sin 2\chi}{\sin^2\eta \cos^2 2\chi} \end{bmatrix}. \quad (\text{B.71})$$

The Metric Tensor

The forms for S and \mathfrak{m} given by Equation (3.33) and Equation (3.31), respectively, lead to the following general form for the metric tensor:

$$(g_{ij}) = \begin{bmatrix} (\partial X_c)' (\partial X_c) & & & \\ & (\partial \rho)' (\partial \rho) & & \\ & & \bar{\omega}' J \bar{\omega} & \bar{\omega}' E \bar{u} \\ & & \bar{u}' E \bar{\omega} & (\bar{u}' J \bar{u} + \bar{v}' \Lambda \bar{v}) \end{bmatrix}. \quad (\text{B.72})$$

The total mass has been assumed to be unity in this expression.

The two third-order matrices, $(\partial X_c)' (\partial X_c)$ and $(\partial \rho)' (\partial \rho)$, are easily calculated. For rectangular center-of-mass coordinates the first is the unit matrix. The second matrix is given by Equation (B.66).

The matrix $\bar{\omega}' J \bar{\omega}$ may be calculated from Equation (B.58) and Equation (B.68) to yield the following:

$$\begin{aligned}
 \bar{\omega}' J \bar{\omega} = & \frac{\rho^2(1+\cos^2\eta)}{4} \begin{bmatrix} \sin^2\beta \\ 1 \\ 0 \end{bmatrix} - \frac{\rho^2\sin^2\eta \cos 2\chi}{2} \begin{bmatrix} \cos 2\gamma \sin^2\beta & \cos 2\gamma \sin \beta & 0 \\ \sin 2\gamma \sin \beta & \cos 2\gamma & 0 \\ 0 & 0 & 0 \end{bmatrix} \\
 & + \rho^2\sin^2\eta \begin{bmatrix} \cos^2\beta & 0 & \cos \beta \\ 0 & 0 & 0 \\ \cos \beta & 0 & 1 \end{bmatrix}. \tag{B.73}
 \end{aligned}$$

APPENDIX C

EXPANSION OF THE COULOMB POTENTIAL

The Coulomb potential may be expanded into a series of harmonic terms. For this, the expressions for the interparticle distances are required. From Equation (2.29) or, more explicitly, from Equation (B.29) it may be shown that the distance between particle i and particle j is given by:

$$r_{ij} = \rho \sqrt{\frac{m_i + m_j}{2m_i m_j}} (1 + \cos 2\chi \cos 2(\gamma' + \delta_{ij}))^{\frac{1}{2}}. \quad (\text{C.1})$$

The δ_{ij} 's which appear in Equation (C.1) must satisfy the condition

$$\tan(\delta_{ij} - \delta_{jk}) = - \sqrt{\frac{m_j}{m_i m_k}}, \quad (\text{C.2})$$

wherein i , j , and k are an even permutation of 1, 2, and 3. Equation (C.2) defines only the differences between the angles. This reflects the fact that the relation is invariant with respect to orthogonal kinematic transformations. For the particular cluster graph chosen in Appendix B the angle δ_{12} vanishes. Equation (C.2) then defines the other two angles uniquely.

The expansion of the Coulomb potential of a single interacting pair into a harmonic series reduces to the expansion of the last factor on the right of Equation (C.1). The binomial expansion may be applied to obtain the following:

$$(1 + \cos 2X \cos 2(\gamma' + \delta))^{\frac{1}{2}} = \sum_{s=0}^{\infty} \frac{\Gamma(\frac{1}{2})}{s! \Gamma(\frac{1}{2} - s)} \cos^s 2X \cos^s 2(\gamma' + \delta) . \quad (C.3)$$

This is also expanded in a harmonic series of the following form

$$(1 + \cos 2X \cos 2(\gamma' + \delta))^{\frac{1}{2}} = \sum_{\lambda\nu} A_{\lambda\nu} d_{\nu/2, \nu/2}^{\lambda/2}(4X) \exp(i2\nu\gamma') . \quad (C.4)$$

The expansion coefficients $A_{\lambda\nu}$ are then found by equating the right hand side of Equation (C.3) with that of Equation (C.4) and integrating over the ranges of definition.

The resulting form of the expansion coefficients is

$$A_{\lambda\nu} = A_{\lambda} \exp(i2\nu\delta) , \quad (C.5)$$

where the coefficient A_{λ} is given by the following series

$$A_{\lambda} = \left(-\frac{1}{8}\right)^{\lambda} (\lambda + 1) \sum_{n=0}^{\infty} \frac{(2\lambda + 4n)! 2^{-6n}}{n!(n + \lambda + 1)!(\lambda + 2n)!} . \quad (C.6)$$

This series may be shown to converge by using Gauss's test (Bromwich 1949). The convergence is very slow, however. The series has been summed on a digital computer. The results are given in Table IV. The value of the first term is known (Zickendraht 1965) to be

$$A_0 = 2^{7/2}/(3\pi) . \quad (C.7)$$

This value was used to get some estimate of the accuracy of the series, at least for the first few coefficients.

The Coulomb potential due to three interacting particles characterized by Z_1 , Z_2 , and Z_3 may now be written in the form of a series of harmonics, such as on the right of Equation (C.4). The coefficients

TABLE IV
VALUES OF THE COULOMB EXPANSION COEFFICIENT A_λ

λ	A_λ
0	1.20041 8
1	-0.48016 6
2	0.30867 7
3	-0.22864 9
4	0.18188
5	-0.15110
6	0.12927
7	-0.11298
8	0.10034
9	-0.09025
10	0.08201
11	-0.07515
12	0.06935
13	-0.06438
14	0.06008
15	-0.05632
16	0.05300
17	-0.05005
18	0.04741
19	-0.04504
20	0.04289
21	-0.04094

NOTE: The accuracy of the above values for A_λ after the first one is not known, but it is believed to be of an order consistent with the number of places shown.

are then of the form

$$A_{\lambda\nu} = A_{\lambda} \alpha \varphi^{-1} (Z_1 Z_2 \sqrt{2\mu_{12}} \exp(2i\nu \delta_{12}) + \dots) . \quad (\text{C.8})$$

The sum in this Equation (C.8) is over the three terms obtained from one another by permuting the indices. The energy is given in mass units. The total mass is assumed to be unity and μ_{ij} is the reduced mass of particles i and j . The fine structure constant is denoted by α .

APPENDIX D

THE COMPUTER PROGRAM QM3BODY

The computer program QM3BODY and its subroutines follow in FORTRAN language after a brief description of the required input cards. Standard library subroutines have been omitted. The input data cards are five in number.

CARD 1 contains the masses M_1 , M_2 , M_3 of the three particles. An optional input quantity is MASSUNIT which is an eight-letter name which specifies the unit of mass used. The format statement is `FORMAT(3E20.0, A8)`.

CARD 2 contains the charges Z_1 , Z_2 , Z_3 of the three particles in units of the electronic charge. Following these three is the maximum order MAXLAM used in the expansion of the potential. Ordinarily, this is twice the order MAXLAMDA used in the expansion of the wave function and given on CARD 4 below. The format statement is `FORMAT(3E20.0, I10)`.

CARD 3 contains the inner boundary point R_0 (usually zero), the match point RMATCH, and the outer boundary point RFINAL. The unit of length is the Compton length associated with the unit of mass chosen above on CARD 1. The corresponding format statement is `FORMAT(3E20.0)`.

CARD 4 contains the maximum order MAXLAMDA used in the harmonic expansion of the wave function, the number MESH1 of intervals between R_0 and RMATCH, the number MESH2 of intervals between RMATCH and RFINAL, and an instruction ITAPE40, which is zero or blank if this is an initial

run, and nonzero if a tape for tape unit 40 has been saved from a previous run. The format statement is `FORMAT(4I10)`.

CARD 5 contains the initial "guessed" energy `ENERGYO` in the unit of mass used on CARD 1, a relative convergence criterion `EPSI`, the number of zeroes `NZEROES` to be expected in the wave function, and the maximum number of iterations `MAXIT` to be allowed in converging toward the energy eigenvalue. The program stops after the maximum number of iterations has been reached or after the relative energy correction becomes less than `EPSI`. The format statement is `FORMAT(2E15.8, 2I10)`.

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PROGRAM QM3BODY
COMMON WEIGHT(87)
COMMON /INPUT/R0,RMATCH,RFINAL,MESH1,MESH2
COMMON /PARAMTRS/ MAXLAMDA, MAXLAM2, NMAX, NUMAX, NMAX1, NUMAX1,
MMAX1, MUMAX1, MUMAXISQ
COMMON/ENERGY/ENERGY0, ENERGY, AMASS, BMASS, CMASS
COMMON /POTENTIAL/ AMASSPR, BMASSPR, CMASSPR, ABCMASS, POT(20)
COMMON /S/ LSU, LSI, LSITWO, LS2, LS, LSTOTAL, INITIALS, S(5000)
COMMON/VECTORS/N1,U1(86),N2,U2(86),V(86)
COMMON / PHI/ N, NZEROS, PHISGN, PHI(15000)
C READ IN INPUT DATA.
C MASSES IN ARBITRARY MASS UNIT. ENERGY IN THE SAME MASS UNIT. LENGT
C HS IN COMPTON WAVELENGTHS(SLASHED) OF THAT MASS UNIT.
ITIME0= ICLOCKF(ITIME)
REWIND 40
REWIND 10
6 CONTINUE
READ 20,AMASS,BMASS,CMASS, MASSUNIT
20 FORMAT (3E20,00, A8)
ABCMASS=AMASS+BMASS+CMASS
AMASSPR=AMASS/ABCMASS
BMASSPR=BMASS/ABCMASS
CMASSPR=CMASS/ABCMASS
IDATE = IDATEF(IDATE)
7 CONTINUE
PRINT (00), IDATE, AMASSPR, BMASSPR, CMASSPR, AMASS, MASSUNIT,
(BMASS, MASSUNIT, CMASS, MASSUNIT, ABCMASS, MASSUNIT
1001 FORMAT(20X16HQM3BODY RESULTS4X5HDATE A8, //27HKPARTICLE MASSES (R
RELATIVE) F21,11, 2F30,11// 27H PARTICLE MASSES (ABSOLUTE) E24,10,
21X A8, 2(E21,10, 1X A8)// 21H TOTAL MASS OF SYSTEM 6X E24,10,1X A8
3// 34HNAME AND DESCRIPTION OF P3TENTIAL )
CALL POTDATA
8 CONTINUE
READ 20,R0,RMATCH,RFINAL
9 CONTINUE
READ 10, MAXLAMDA, MESH1, MESH2, ITAPE40
10 FORMAT (4I10)
NMAX = MAXLAMDA/2
NMAX1=NMAX+1
LS0=(NMAX1+1)*NMAX1/2
NUMAX = (MAXLAMDA + 1)/2
NUMAX1=NUMAX+1
MMAX1=NMAX1*NUMAX
LS1=MMAX1*NMAX1
LSITWO = LS1 + LS1
LS2=(MMAX1+1)*MMAX1/2
LS = LS2*4 + LSITWO + LS0
LSTOTAL = 4999
MAXLAM2 = MAXLAMDA + MAXLAMDA
MOMAX1=NMAX1+MMAX1+MMAX1
MOMAXISQ=MOMAX1*MOMAX1
MUPPER=MOMAXISQ+1
T = RC/(R0+(RMATCH - R0) / MESH1)
TSO = T*T
TR0T = SQRTF(T)
MOMAX2 = MOMAX1 + 1
IJUMP = MOMAX2*MMAX1
IWO = 0
WI = 0,0
IWI = NMAX1
DO 2026 I=0, MAXLAMDA
WI = WI + 1,0
WO = 1,0/WI
NU = -L
IF(NU) 2026, 2027, 2026
2026 IWI = IWI + 1

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      IW2 = IW1 + NMAXI
      WEIGHT(IW1) = W0
      WEIGHT(IW2) = WEIGHT(IW1)
      NU = NU + 2
      IF(NU) 2026, 2027, 2028
2027 IW0 = IW0 + 1
      WEIGHT(IW0) = W0
2028 CONTINUE
      IF(ITAPE40) 12, 14
      14 CALL TAPEMATE
      15 CONTINUE
      PRINT 1006, RU, RMATCH, RFINAL, MESH1, MESH2
1006 FORMAT (16HBOUNDARY POINTS 11X 3E25.10 / 30H NUMBER OF INTERVALS
1IN MESHES 3X 2I25//)
      PRINT 1007, MAXLAM2, NMAXI, MMAXI, MUMAXI, LSO, LSI, LS2, LS
1007 FORMAT(71HKSIX DIMENSIONAL SPHERICAL HARMONICS TERMINATED AT ORDER
1 L = 2*LAMBDA = 13, 1H, / 70H THE CORRESPONDING DIMENSION OF THE E
2XPANSION COEFFICIENTS VECTOR IS ( 13, 5H + 2* 13, 3H) = 13 / 68H
3 THE POTENTIAL MATRIX IS CHARACTERIZED BY LS = LSO + 2*LS1 + 4*LS2
4 = 13, 5H + 2* 14, 5H + 4* 14, 2H = 15, 1H,/)
      19 CONTINUE
      SCALE1 = 1, E-100
      SCALER1 = 1, E-10
      SCALE2 = 1, E-100
      SCALER2 = 1, E-10
      READ 11, ENERGY0, EPS1, NZEROS, MAXIT, ISCALE, NTRY, IREPEAT0
      11 FORMAT (2E15.0, 5I10)
      IF (MAXIT) 12, 13, 13
      12 IT = -MAXIT
      GO TO (9, 8, /, 6), IT
      13 CONTINUE
      IF (ISCALE) 16, 18, 10
      16 READ 17, SCALE1, SCALER1, SCALE2, SCALER2
      17 FORMAT (4E10.3)
      18 CONTINUE
      PRINT 1008, IREPEAT0, MAXIT, EPS1, SCALE1, SCALER1, SCALE2, SCALER2
1008 FORMAT (16HINPUT ASKED FOR 15, 22H REPEATS, NO MORE THAN 15, 52H
1ITERATIONS AND A CONVERGENCE CRITERION OF EPSILON = E10.3, 1H, //
223H SCALE FACTORS USED ARE / 25X 8HSCALE1 = E10.3, 10X 9HSCALER1 =
3E10.3/ 25X 8HSCALE2 = E10.3, 10X 9HSCALER2 = E10.3//)
      ENERGY=ENERGY0*ABCMASS
      ENINC = ENERGY
      IF(ENINC) 2020, 2021, 2022
2021 ENINC = -0.005
2020 ENINC = -ENINC
2022 CONTINUE
      IT = MAXIT
      NI = 1
      DO 20 J= 1, MUMAXI
      20 UI(J) = 0.0
      N2=0
      UNAX2=0.0
      UMAX1=0.0
      PRINT 1009, ENERGY0
1009 FORMAT (23HINITIAL ENERGY ASSUMED 35X E25.10.5H (N))
C ALPHA
      24 IREPEAT = IREPEAT0
C THIS IS STARTING POINT OF ITERATIONS GOVERNED BY
C INDEX REPEAT AND GOVERNED BY ENERGY EIGENVALUE CONVERGENCE,
      25 NO=MUMAXI
      INITIALS=0 $ CALL MATCHIRL
      SINTEGRL=0.0
C SET BOUNDARY CONDITIONS ON THE LEFT
      CALL DIAGONAL(PHI(1),MUMAXI,0.0)
      CALL DIAGONAL(PHI(MUPPER),MUMAXI,1.0)
      J1 = NMAXI

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J = 0
TPR = TROOT
IPHI0 = 1
IPHI1 = NMAX*(MOMAX2) + 1
JDELTA = (N1-1)*MOMAX1
DO 2004 L = 0, MAXLAMDA
  TPR = TPR*TSQ
  DO 2005 NU = 1, J
    IPHI1 = IPHI1 + MOMAX2
    IPHI2 = IPHI1 + IJUMP
    PHI(IPHI1) = TPR
    PHI(IPHI2) = PHI(IPHI1)
    J1 = J1 + 1
    J1P = J1 + JDELTA
    J1PR = J1P + MOMAX1SQ
    J2PR = J1PR + MMAX1
    J2P = J2PR - MOMAX1SQ
    J2 = J2P - JDELTA
    IF (U1(J1)) 2005, 2006
2005 PHI(J1PR) = U1(J1)
    PHI(J1P) = PHI(J1PR) * TPR
2006 IF (U1(J2)) 2007, 2003
2007 PHI(J2PR) = U1(J2)
    PHI(J2P) = PHI(J2PR)*TPR
2003 CONTINUE
    IF ((L/2)*2 - L) 2004, 2001
2001 PHI(IPHI0) = TPR
    IPHI0 = IPHI0 + MOMAX2
    J = J+1
    JP = J + JDELTA
    JPR = JP + MOMAX1SQ
    IF (U1(J)) 2002, 2004
2002 PHI(JPR) = U1(J)
    PHI(JP) = PHI(JPR)*TPR
2004 CONTINUE
C          CALCULATE MATRIX W OF WAVE FUNCTIONS ON THE LEFT
C          UP TO MATCH POINT.
40 CALL PHIMAKER(R0,RMATCH,MESH1,SINTEGRL,N0,1)
   K=MUPPER
   I=1
   IF (-N0)42,42,51
41 I=MUPPER      $ K=I
42 I=I+MUMAX1SQ $ KI=K-I+MOMAX1SQ
C          STORE W ON TAPE.
   WRITE TAPE 10,(PHI(J),J=K,KI)
   DO 45 J=I,I
45 PHI(J)=PHI(J)+PHI(K)
   FMESH=MESH1
   H=(RMATCH-R0)/FMESH
   R2=H+NMATCH
   R1=RMATCH-H
   HRECIP1=0.5/H
C          CALCULATE W' AND STORE ON TAPE.
   CALL PHIMAKER(R1,R2,2,SINTEGRL,N0,1)
   DO 55 J=I,I
55 PHI(J)=PHI(J)*HRECIP1
   WRITE TAPE 10,(PHI(J),J=I,I)
C          CALCULATE THE TRANSPOSE OF W*HRECIP AND STORE ON TAPE.
   CALL TRANSPOZ(PHI(I),MOMAX1)
   CALL TRANSPOZ(PHI(MUPPER),MUMAX1)
   DI = SCALE1
   CALL MATO(PHI(K),PHI(I),MOMAX1,MOMAX1,DI,SCALE1,MOMAX1,MOMAX1)
   IF (DI)61,60
60 CALL STOP(501)
61 WRITE TAPE 10,(PHI(J),J=I,I)
   N0=MOMAX1

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C          SET BOUNDARY CONDITIONS ON THE RIGHT.
CALL DIAGONAL(PHI(1),MOMAXI,0,0)
CALL DIAGONAL(PHI(MUPPER),MOMAXI,1,0)
IF(N2)70,75
70 J=(N2-1)*MOMAXI+MUPPER
DO 72 I=1,MOMAXI
PHI(J) = PHI(J) + U2(I)
72 J=J+1
C          CALCULATE R AND STORE ON TAPE.
75 CONTINUE
CALL PHIMAKER(RFINAL,RMATCH,MESH2,SINTEGR,NO,1)
K=MUPPER
I=1
IF(-NO)82,82,81
81 I=MUPPER      $ K=1
82 II=I+MOMAXISQ-1  $ KI=K+MOMAXISQ-1
WRITE TAPE 10,(PHI(J),J=K,KI)
DO 85 J=I,II
85 PHI(J)=PHI(J)+PHI(J)
FMESH=MESH2
H=(RFINAL-RMATCH)/FMESH
R3=H+RMATCH
R4=RMATCH-H
HRECIP2=0.5/H
C          CALCULATE R' AND STORE ON TAPE.
CALL PHIMAKER(R3,R4,2,SINTEGR,NO,1)
DO 95 J=I,II
95 PHI(J)=PHI(J)*HRECIP2
WRITE TAPE 10,(PHI(J),J=I,II)
BACKSPACE 10
C          CALCULATE (R+HRECIP - W*HRECIP) AND FIND ITS MINIMUM
C          EIGENVALUE AND CORRESPONDING EIGENSOLUTION V.
CALL TRANSPOZ(PHI(1),MOMAXI)  $ BACKSPACE 10
CALL TRANSPOZ(PHI(MUPPER),MOMAXI)
BACKSPACE 10
D2 = SCALE2
CALL MATQ(PHI(K),PHI(II),MOMAXI,MOMAXI,D2,SCALER2,MOMAXI,MOMAXI)
IF(D2)101,100
100 CALL STOP(510)
101 KI=K+MOMAXISQ-1
READ TAPE 10,(PHI(J),J=K,KI)
DO 110 J=1,MOMAXISQ
110 PHI(J)=PHI(J) + PHI(J+MOMAXISQ)
CALL TRANSPOZ(PHI(1),MOMAXI)
EIGEN=0,0
N = 20
CALL MINEIG (PHI,V,MOMAXI,NTRY, N,0,5E-9,EIGEN,PHI(MUPPER))
REWIND 40
BUFFER IN (40, 1) (S(1), S(LS))
REWIND 40
D=PHI(MUPPER)
C          CALCULATE STARTING VECTORS U1 AND U2.
READ TAPE 10,(PHI(J),J=1,MOMAXISQ)  $ REWIND 10
I = MUPPER
DO 111 J = 1, MOMAXI
PHI(I) = V(J)
111 I = I + 1
UMAX2 = SCALE2
CALL UVECTOR(U2,PHI(MUPPER),PHI,N2,MOMAXI,UMAX2,SCALER2)
READ TAPE 10,(PHI(J),J=1,MOMAXISQ)
I = MUPPER
DO 112 J = 1, MOMAXI
PHI(I) = V(J)
112 I = I + 1
UMAX1 = SCALE1
CALL UVECTOR(U1,PHI(MUPPER),PHI,N1,MOMAXI,UMAX1,SCALER1)

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REWIND 10
IREPEAT=IREPEAT-1
IF (IREPEAT) 120, 120, 25
C THIS IS THE END POINT OF ITERATIONS GOVERNED BY INDEX IREPEAT
120 SINTEGRL=0.5E-38
SCALE = UMAX1/UMAX2
INITIALS=0 $ CALL MATCNTRL
NO=1
TPR = TROOT
J = 0
JI = MMAX1
UI(N1) = 1.0
DO 2014 L = 0, MAXLAMDA
TPR = TPR*TSO
DO 2013 NO = 1, J
JI = JI + 1
J1PR = JI + MMAX1SQ
J2PR = J1PR + MMAX1
J2 = J2PR - MMAX1SQ
PHI(J1PR) = UI(JI)
PHI(J1) = PHI(J1PR)*TPR
PHI(J2PR) = UI(J2)
PHI(J2) = PHI(J2PR)*TPR
2013 CONTINUE
IF((L/2)*2-L) 2014, 2011
2011 J = J+1
JPR = J + MMAX1SQ
PHI(JPR) = UI(J)
PHI(J) = PHI(JPR)*TPR
2014 CONTINUE
UI(N1) = 0.0
NZEROES = 0
PHISGN = 0.0
CALL PHIMAKER(R0,RMATCH,MESH1,SINTEGRL,NO,1)
K=MMAX1SQ
I=0
IF(=NO) 142,142,141
141 I=MMAX1SQ $ K=0
142 II=I+MMAX1-1
DO 145 J=1,II
145 PHI(J+1)=PHI(J+1)+PHI(J+1)
SINTEGRL = SINTEGRL + SINTEGRL
CALL PHIMAKER(R1,R2,2,SINTEGRL,NO,1)
LOVE=MMAX1
IF(LOVE-1) 150,150
150 LOVE=2
155 LOVEYGL=LOVE+MMAX1SQ
C PHI- GOES TO M/MAXI + 1, ETC.
C PHI- PRIME GOES TO M/MAXI + 1 + M/MAX1SQ, ETC.
DO 160 J=1,MMAX1
PHI(LOVE+J)=PHI(K+J)
160 PHI(LOVEYGL+J)=PHI(I+J)*HRECIP1
NO=1
SINTEGRL = SCALE*SCALE*SINTEGRL*0.5
DO 170 J=1,MMAX1
PHI(J)=0.0
170 PHI(J+MMAX1SQ)=U2(J)
PHI(N2+MMAX1SQ)=1.0
PHISGN = 0.0
CALL PHIMAKER(RFINAL,RMATCH,MESH2,SINTEGRL,NO,1)
K=MMAX1SQ
I=0
IF(=NO) 185,185,180
180 I=MMAX1SQ
K=0
185 II=I+MMAX1-1

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      DO 190 J=1,11
190  PHI(J+1)=PHI(J+1)+PHI(J+1)
      SINTEGRL = SINTEGRL + SINTEGRL
      CALL PHIMAKER(R3,R4,2,SINTEGRL,NO,1)
      REWIND 40
      BUFFER IN (40, 1) (S(1), S(LS))
      REWIND 40
      C=0.0
      DO 200 J=1,MMAXI
      PHI(I+J) = -PHI(I+J)*HRECIP2
      C = PHI(I+J)*PHI(LOVE+J)*WEIGHT(J) - C
200  C = PHI(K+J)*PHI(LOVEY0+J)*WEIGHT(J) - C
      T1=ENERGY/ABCMASS
      DELTA = C*SCALE/SINTEGRL
      SNEW = +1.
      IF(NZERGES-NZEROS) 2031, 2032, 2030
2030  SNEW = -1.
2031  IF(SNEW*SOLD) 2041, 2041, 2040
2040  ENINC = 1.5*ENINC
      GO TO 2045
2041  ENINC = 0.5*ENINC
2045  DELE = ENINC*SNEW
      SOLD = SNEW
      GO TO 2030
2032  SOLD = 0.0
      DELE = DELTA
      ENINC = DELE
      IF(ENINC) 2034, 2033, 2050
2033  ENINC = -.005
2034  ENINC = -ENINC
2050  CONTINUE
      ENERGY = ENERGY + DELE
      T2=ENERGY/ABCMASS
      T3=DELTA/ABCMASS
      ITIME = (ICLOCKF(ITIMEC) - ITIME0)/60
      DET = PRODUCT(D, D1)
      DET = PRODUCT(DET, D2)
      PRINT 1016, ITIME, T3, T2, N, DET, NZERGES
1016  FORMAT (7H TIME = I5, 4H SEC 4X 12H CORRECTION = E17.10, 4X 13H NEXT
1  ENERGY = E17.10, 14, 3X 13H DETERMINANT = E17.10/ 40X 1/H WAVE FUNC
2  TION HAS I5, 8H ZERGES,/)
      T = T2
      IF (T) 220, 220, 210
210  T = -T
220  IF (T+T1) 240, 260, 230
230  T = -T1
240  IF (T-T1) 260, 260, 250
250  T = T1
260  T4 = T3
      IF (T4) 280, 300, 270
270  T4 = -T4
280  IF (T4/T - EPS1) 300, 300, 290
290  IT = IT - 1
      IF (IT) 300, 300, 24
300  CONTINUE
      CALL STOP(550)
      PRINT 310
310  FORMAT (1H2)
      GO TO 19
      END QMSBODY
      SUBROUTINE POTENCHL
C  THE COULOMB POTENTIAL BETWEEN THREE PARTICLES.
C  POT(1) CONTAINS POT., POT(2) CONTAINS POT1.
C  POT(3) CONTAINS THE CONSTANT FOR A GIVEN R,
C  POT(4) CONTAINS CONSTANT.
      COMMON /POTENCHL/ AMASSPR, BMASSPR, CMASSPR, ABCMASS, POT(20)

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COMMON / INCOUL / VNU(36), VNU(36)
COMMON / R / R, T=CHSQ
COMMON / COEFIF / LPR, LPRPR, L, NUPR, NUPRPR, NU, CDEF, RECLAM1, FACLOG(300)
EQUIVALENCE (Z1, POT(5)), (Z2, POT(6)), (Z3, POT(7))
EQUIVALENCE (POT1, POT(2))
DATA (ALPHA = 0.00729725)
DATA (COUL = 1.2004217549, -.47970460639, .308224, -.228199, .18188
1, -.1511, 0.1293, -.1130, .10035, -.09025, .08201, -.07515, .06935,
2, -.06438, .06008, -.05632, .05300, -.05005, .04741, -.04504,
3, .04289, -.04094, .0, .0, .0, .0, .0, .0, .0, .0)
DIMENSION COUL(30)
C ASSUMES NUPRPR IS POSITIVE AND NOT GREATER THAN LPRPR,
IF(LMAX-LPRPR) 20, 10, 10
10 TEMP = POT(3)*COUL(LPRPR+1)
POT = TEMP*VNU(NUPRPR+1)
POT1 = TEMP*VNU(NUPRPR+1)
RETURN
20 POT = 0.0
POT1 = POT
RETURN
ENTRY POTPREP
POT(3) = POT(5)/R
RETURN
ENTRY POTDATA
100 READ 100, Z1, Z2, Z3, LMAX
FORMAT(3E20,00, 2I10)
POT(4) = AECMASS*ALPHA
PRINT 200, LMAX, Z1, AMASSPR, Z2, BMASSPR, Z3, CMASSPR
200 FORMAT(/40X 21HTHE COULOMB POTENTIAL / 40X 24HTRUNCATED TO LAMBDA
1 = 0, 15 / 40X 22HCHARGES AND MASSES ARE / 3(40X 2F25.10)/)
CALL INCOUL(LMAX)
PRINT 400, ((1, VNU(I+1), VNU(I+1), COUL(I+1)), I=0, LMAX)
400 FORMAT( 8X 2HN0 28X 7HVNUREAL 23X 12HVNUMAGINARY 26X 7HCOULCON
1//5X 15, 16X E17.10, 18X E17.10, 18X E17.10//)
500 RETURN
END

SUBROUTINE PHIMAKER(RO,RFINAL,MESHPTS,SINTEGRL,NO,INITCOL)
COMMON WEIGHT(87)
COMMON/ENERGY/ENERGY0, ENERGY, AMASS, BMASS, CMASS
EQUIVALENCE (ENERGY, ENVERHSQ)
EQUIVALENCE (LS2, LS3)
COMMON / PHI / N, NZERDES, PHISGN, PHI(15000)
COMMON /S/ LSO, LSI, LSI1K0, LS2, LS, LSTOTAL, INITIALS, S(5000)
COMMON/ PRAMTRS/ MAXLAMDA, MAXLAM2, NMAX, NUMAX, NMAX1, NUMAX1,
1MMAX1, NOMAX1, MOMAXISQ
C THE PARAMETERS ARE DEFINED AS FOLLOWS.
C NMAX1=NMAX+1
C NUMAX1=NUMAX+1
C MMAX1=MMAX1*NUMAX
C MOMAXISQ=MMAX1+MMAX1+MMAX1
C MOMAXISQ=MOMAX1*MOMAX1
C LSO=(NMAX1+1)*NMAX1/2
C LSI=MMAX1*MMAX1
C LS2=(MMAX1+1)*MMAX1/2
C THE MAGNITUDE OF NO IS THE NUMBER OF COLUMN VECTORS
C IN EACH PHI MATRIX, THE SIGN IS POSITIVE (NEGATIVE)
C IF THE LAST PHI CALCULATED WAS STORED IN
C UPPER (LOWER) PHI, I.E., PHI(MOMAXISQ+J)(PHI(J)).
C SIGMA = 0.0
MDELTA=MOMAXISQ
MIN=(INITCOL-1)*MOMAX1+1
IF(=NO)30,600,20
20 MDELTA=-MOMAXISQ
MIN=MOMAXISQ+MIN
NO=NO

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30 MAX=MIN+(NC+1)*MOMAXI
   FMESHPTS=MESHPTS
   FMESHPT=0.0
   IF (MESHPTS)51,51,50
50 SIGN=1.0
   DELTAR=RFINAL-RQ
   IF (DELTAR)54,55,56
55 CALL STOP(101)
51 CALL STOP(102)
54 DELTAR=-DELTAR
   SIGN=-1.0
56 H=DELTAR/FMESHPTS
   TWOHSQ = H*H*2.0
   CONSTH4 = TWOHSQ * TWOHSQ * 0.0625
   ECONST = (-E0VERHSQ) * TWOHSQ + 2.0
   DO 300 MESHPT=2,MESHPTS
   FMESHPT=1.0+FMESHPT
   MAX=MAX+MDELTA
   MIN=MIN+MDELTA
   MDELTA=-MDELTA
   INITIALS=INITIALS+LS
   IF (INITIALS-LS-1)59,61
59 IF (INITIALS+LS-1-LSITOTAL)61,61,60
60 INITIALS=1
61 CALL MATCHNTRL
CALCULATE AND PREPARE ADDRESSES
R=(FMESHPT-FMESHPTS)*SIGN*H*RFINAL
HRSQ = (H*R)**2
HOLD = HRSQ*ECONST + CONSTH4
HRSQREC = 1./HRSQ
INIT3 = INITIALS + LSO + 2*LS1
DO 200 M02P=MIN,MAX,MOMAXI
J0 = M02P
M12P = J0 + MMAX1
M12 = M12P - 1
J = M12
M22 = J + MMAX1
M22M = M22 - 1
M22P = M22M + 2
IADDRESS = M22P + INIT3
M32 = M22 + MMAX1
M02 = M32 - MOMAXI
M02P1 = M02 + 2
M03P1 = M02P1 + MDELTA
IS = INITIALS
IADDRESS = IS + LSO
FLAMDA1 = 0.0
DO 100 LAMDA = 0, MAXLAMDA
FLAMDA1 = FLAMDA1 + TWOHSQ
PHIMULT = (HOLD/FLAMDA1 + FLAMDA1) * HRSQREC
NU = LAMDA
IF (NU) 100, 80, 90
CALCULATE PHI-REAL AND PHI-IMAGINARY,
90 J = J+1
   JPR = J + MDELTA
   JPRI = JPR + MMAX1
   JI = JPRI + MDELTA
   T3 = 0.0
   T3I = T3
   DO 97 I= M02P, M12
   IADDRESS = IADDRESS + 1
   IADDRESS2 = IADDRESS + LS1
   T3 = S(IADDRESS-1)*PHI(I) + T3
   T3I = S(IADDRESS2-1)*PHI(I) + T3I
97 CONTINUE
   IPR = M22

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DO 98 I = M12P, J
IPR = IPR + 1
IADDRESS0 = IPR + IADDRESS
IADDRESS1 = IADDRESS0 + LS3
IADDRESS2 = IADDRESS1 + LS3
IADDRESS3 = IADDRESS2 + LS3
T3 = S(IADDRESS0) * PHI(I) + S(IADDRESS1) * PHI(IPR) + T3
T31 = S(IADDRESS2) * PHI(I) + S(IADDRESS3) * PHI(IPR) + T31
98 CONTINUE
IADDRE = M22 - IADDRESS0
DO 99 I = J, M22M
IPR = IPR + 1
IADDRESS0 = IPR + IADDRESS0 - M22P
IADDRESS1 = IADDRESS0 + LS3
IADDRESS2 = IADDRESS1 + LS3
IADDRESS3 = IADDRESS2 + LS3
T3 = S(IADDRESS0) * PHI(I+1) + S(IADDRESS1) * PHI(IPR) + T3
T31 = S(IADDRESS2) * PHI(I+1) + S(IADDRESS3) * PHI(IPR) + T31
99 CONTINUE
PHI(JPR) = (PHI(J) * PHIMULT + T3) * FLAMDAI - PHI(JPR)
PHI(JPRI) = (PHI(JI) * PHIMULT + T31) * FLAMDAI - PHI(JPRI)
NU = NU - 2
IF (NU) 100, 80, 90
C THE CALCULATION OF PHIC.
80 J0 = J0 + 1
JOPR = J0 + MDELTA
L = JOPR - M03PI
T3 = 0.0
DO 85 I = M02PI, J0
IS = IS + 1
T3 = S(IS-1) * PHI(I-1) + T3
85 CONTINUE
IT = IS
DO 87 I = J0, M12
L = L+1
IT = L+IT
T3 = S(IT-1) * PHI(I) + T3
87 CONTINUE
IBAR = M22M
DO 88 I = M12, M22M
IBAR = IBAR + 1
IT = IT + MMAXI
ITBAR = IT + LSI
88 T3 = S(IT-1)*PHI(I+1) + S(ITBAR-1)*PHI(IPR+1) + T3
PHI(JOPR-1) = (PHI(J0-1) * PHIMULT + T3) * FLAMDAI - PHI(JOPR - 1)
100 CONTINUE
CALCULATE SINTEGRAL
IF(SINTEGRAL)140,200
200 CALL MATCHNRL
300 CONTINUE$GG TO 500
140 IW = 1
DO 150 I = M02P, M32
SIGMA = PHI(I)*PHI(I)*WEIGHT(IW) + SIGMA
150 IW = IW + 1
PHINE = PHI(M02 + N)
IF (PHINE*PHISGN) 155, 157, 200
155 NZERGES = NZERGES + 1
157 IF(PHINE) 160, 200, 159
159 PHISGN = 1.0
GO TO 200
160 CONTINUE
PHISGN = -1.0
GO TO 200
350 CALL STOP(103)
500 IF(=MDELTA)600,350,550
550 NO=-NO

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600 SINTEGRL = SIGMA*H + SINTEGRL
RETURN
END
SUBROUTINE TAPEMATE
COMMON / R / R, TWOHSQ
COMMON / COEF / LPR, LPRPR, L, NUPR, NUPRPR, NU, CREF, RECLAMI, FACLOG(300)
COMMON / S / LSD, LSI, LSI TWO, LS2, LS, LSTOTAL, INITIALS, S(5000)
EQUIVALENCE (INITIALS, NDIFF)
COMMON / INPUT / RO, RMATCH, RFINAL, MESH1, MESH2
FACLOG(1) = 0.0
FACLOG(2) = FACLOG(1)
FN = 1.0
DO 10 N = 3, 300
FN = FN * 1.0
10 FACLOG(N) = LOGF(FN) + FACLOG(N-1)
CALL TAPERST
NDIFF=0
I=0
NDIFFMAX=LSTOTAL/LS-2
H=(RMATCH-RO)/MESH1
DO 200 MESHPT=1, MESH1
R=(MESH1-MESHPT)*(-H)+RMATCH
50 CALL TAPER
IF (NDIFFMAX-NDIFF)50,60,60
60 IF (NDIFF+1)80,70
70 NDIFF=0
80 IF (I+LS-LSTOTAL)110,110,100
100 I=0
110 CALL POTPREP
CALL MATRIX(I)
200 NDIFF=NDIFF+1
H=(RFINAL-RMATCH)/MESH2
DO 400 MESHPT=1, MESH2
R=(MESH2-MESHPT)*H+RMATCH
250 CALL TAPER
IF (NDIFFMAX-NDIFF)250,260,260
260 IF (NDIFF+1)280,270
270 NDIFF=0
280 IF (I+LS-LSTOTAL)310,310,300
300 I=0
310 CALL POTPREP
CALL MATRIX(I)
400 NDIFF=NDIFF+1
450 CALL TAPER
IF (NDIFF+1)450,500
500 CALL TAPERFIN
RETURN
END
SUBROUTINE TAPER
COMMON / S / LSD, LSI, LSI TWO, LS2, LS, LSTOTAL, INITIALS, S(5000)
EQUIVALENCE (INITIALS, NDIFF)
C NDIFF IS THE NUMBER OF MATRIX BLOCKS WHICH HAVE BEEN
COMPLETELY CALCULATED MINUS THE NUMBER WHICH HAVE STARTED TO BE TAPED.
GO TO 20
5 IF(NDIFF)101,101,10
10 NDIFF=NDIFF-1
IFINAL=IFINAL+LS
IF(IFINAL-LSTOTAL)15,15,12
12 IFINAL=LS
15 I=IFINAL-LS+1
19 BUFFER OUT( 40,1)(S(1),S(IFINAL))
20 IF(UNIT, 40)100,5,30,25
25 CALL STOP(401)
30 CALL STOP(402)
ENTRY TAPERST
IFINAL=0

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100 RETURN
101 NDIFF=-1      & RETURN
      ENTRY TAPEFIN
500 END FILE 40
501 REWIND 40
      RETURN
      END
      SUBROUTINE MATRIX (INIT)
      COMMON /POTENCHL/ AMASSPR, BMASSPR, CMASSPR, ABCMASS, POT(20)
      EQUIVALENCE (POT1, POT(2))
      COMMON / R / R, TWOHSQ
      COMMON /COEFIF/ LPR, LPRPR, L, NU, NU, NU, COEF, RECLAM1, FACLOG(300)
      COMMON /PARAMTRS/ MAXLAMDA, MAXLAM2, NMAX, NUMAX, NMAX1, NUMAX1,
      IMAX1, MMAX1, MMAXISO
      COMMON /S/ LSO, LSI, LSITWO, LS2, LS, LSTOTAL, INITIALS, S(5000)
      EQUIVALENCE (NO, NO)
      IO = INIT
      I1 = IO + LSO
      I2 = I1 + LSITWO
      FLAMDAI = 0.0
      DO 999 L = 0, MAXLAMDA
      FLAMDAI = FLAMDAI + 1.0
      RECLAM1 = 1.0/FLAMDAI
      NU = L
      NUTEST = NL
10  L1 = 0
      L2 = L
      LMAX = L2 - 1
      LMIN = LMAX + 2
      LSIGN = 1
20  DO 800 LPR = L1, L2
      LMAX = LMAX + 1
      LMIN = LMIN - LSIGN
      NU = LPR + 2
40  NU = NU - 2
      IF (NU = NUTEST) 50, 50, 40
50  IF (NU) 800, 100, 400
      CALCULATE S2,S AND S3,S,
400 I2 = I2 + 1
      I2I = I2 + LS2
      I3I = I2I + LS2
      I3 = I3I + LS2
      SUM = 0.0
      SUMI = SUM
      SUM3I = SUMI
      SUM3 = SUM3I
      NUPLUS = NU + NU
      NUMINUS = NU - NU
      LPRPR = NUMINUS
      IF (LPRPR = LMIN) 408, 410, 410
408 LPRPR = LMIN
410 IF (LPRPR = NUPLUS) 415, 411, 411
411 NU = NUPLUS
      CALL POTENCHL
      IF (POT) 413, 412
412 IF (POT1) 413, 415
413 NU = -NU
      CALL COEFIF
      SUM3 = COEF * POT + SUM3
      SUM3I = COEF * POT1 + SUM3I
      NU = -NU
415 NU = NUMINUS
      CALL POTENCHL
      IF (POT) 417, 416
416 IF (POT1) 417, 418
417 CALL COEFIF

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```

SUM = COEF*POT + SUM
SUMI = COEF*POTI + SUMI
418 LPRPR = LPRPR + 2
IF (LPRPR-LMAX) 410, 410, 420
420 S(12) = (SUM3 + SUM)
S(12I) = (SUM3I + SUMI)
S(13) = (SUMI + SUM3I)
S(13I) = (SUMI + SUM3I)
S(13) = (SUMI + SUM3I)
GO TO 700
100 IF (NU) 300, 200
CALCULATE S0
200 I0 = I0 + 1
SUM = 0.0
NUPRPR = 0
LPRPR = LMIN
210 CALL POTENCHL
IF (POT) 215, 218
215 CALL COEFIF
SUM = COEF*POT + SUM
218 LPRPR = LPRPR + 4
IF (LPRPR - LMAX) 210, 210, 220
220 S(I0) = SUM
GO TO 700
CALCULATE SI AND SII
300 I1 = I1 + 1
I11 = I1 + LSI
SUM = 0.0
SUMI = SUM
NUPRPR = NL
LPRPR = NU
IF (LPRPR-LMIN) 308, 310, 310
308 LPRPR = LMIN
310 CALL POTENCHL
IF (POT) 315, 312
312 IF (POTI) 315, 318
315 CALL COEFIF
SUM = POT*COEF + SUM
SUMI = POTI*COEF + SUMI
318 LPRPR = LPRPR + 2
IF (LPRPR - LMAX) 310, 310, 320
320 S(I1) = SUM
S(I11) = SUMI
GO TO 700
700 NUPR = NUPR + 2
IF (NUPR) 800, 100, 400
800 CONTINUE
IF (LSIGN) 900, 810, 810
810 LSIGN = -1
NUTEST = LSIGN + NUTEST
LI = L + 1
L2 = MAXLAMDA
GO TO 20
900 NU = NU + 2
NUTEST = NL
IF (NUTEST) 999, 10, 10
999 CONTINUE
INIT = INIT + LS
RETURN
END
SUBROUTINE INCOUL(NUMAX)
EQUIVALENCE(M1, AMASSPR), (M2, BMASSPR), (M3, CMASSPR), (M, ABCMASS)
COMMON /POTENCHL/ AMASSPR, BMASSPR, CMASSPR, ABCMASS, POT(20)
EQUIVALENCE (Z1, POT(5)), (Z2, POT(6)), (Z3, POT(7))
COMMON / INCOUL/ VNU(36), VNUI(36)
TYPE REAL M1, M2, M3, M
A12 = Z1*Z2*SQRT(2.0*M1*M2/(M1 + M2))

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A23 = Z2*Z3*SQRTF(2.0*M2*M3/(M2 + M3))
A10 = A23
ADDIREAL = A10
A31 = Z3*Z1*SQRTF(2.0*M3*M1/(M3+M1))
A20 = A31
ADD2REAL = A20
VNU(1) = ADD2REAL + A23 + A12
ADD1IMAG = 0.0
ADD2IMAG = ADD1IMAG
VNU(1) = ADD2IMAG
FNUI = 1.0
SYMPROD = 4.0*M1*M2*M3
SYMROCT = SQRTF(SYMPROD)
T1 = M1*M3 + M2
IF(T1) 20, 10
10 COS23 = 1.0
TAN23 = 0.0
TAN23SQ = TAN23
GO TO 50
20 T2 = T1 - M2 - M2
IF(T2) 40, 30
30 COS23 = 0.0
TAN23 = COS23
TAN23SQ = TAN23
GO TO 50
40 COS23 = T2/T1
TAN23 = SYMROCT/T2
TAN23SQ = TAN23*TAN23
50 T1 = M2*M3 + M1
IF(T1) 70, 60
60 COS31 = 1.0
TAN31 = 0.0
TAN31SQ = TAN31
GO TO 100
70 T2 = T1 - M1 - M1
IF(T2) 90, 80
80 COS31 = 0.0
TAN31 = COS31
TAN31SQ = TAN31
GO TO 100
90 COS31 = T2/T1
TAN31 = SYMROCT/T2
TAN31SQ = TAN31*TAN31
100 CONTINUE
DO 1000 NU = 1, NUMAX
VREAL = A12
VIMAG = 00.0
IF(COS23) 550, 500
500 T1 = ADDIREAL
ADDIREAL = -ADD1IMAG
VREAL = ADDIREAL + VREAL
ADD1IMAG = T1
VIMAG = ADD1IMAG
550 IF(COS31) 650, 600
600 T2 = ADD2REAL
ADD2REAL = ADD2IMAG
VREAL = ADD2REAL + VREAL
ADD2IMAG = -T2
VIMAG = ADD2IMAG + VIMAG
650 A10 = A10*COS23
A1 = A10
B1 = A1*TAN23
A20 = A20*COS23
A2 = A20
SUM = A2 + A1
AD2 = 0.0

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```

BD2 = AD2
AD1 = *1,5
BD1 = *,5
FNU = FNU1
BNU = FNU
FNU1 = BNU + 1,0
BN1 = FNU1 + 0,5
AN1 = BN1 + 1,0
BN2 = (-FNU1)*FNU*0,25
AN2 = (-FNU1-1,)*FNU1*0,25
ANU = 1,0
LMAX = NU/2
DO 700 L=1, LMAX
A1 = A1*TAN23SQ
A2 = A2*TAN31SQ
ATOTAL = A2 + A1
AD1 = AD1 + 2,0
AD2 = AD1 + AD2
AN1 = AN1 + 2,0
AN2 = AN1 + AN2
ANU = (AN2/AD2)*ANU
SUM = ANU * ATOTAL + SUM
700 CONTINUE
VNU(NU+1) = VREAL + SUM
B2 = A2*TAN31
SUM1 = (B2 + B1)*BNU
LMAX1 = (NU-1)/2
DO 800 L=1, LMAX1
B1 = B1*TAN23SQ
B2 = B2*TAN31SQ
BTOTAL = B2 + B1
BD1 = BD1 + 2,0
BD2 = BD1 + BD2
BN1 = BN1 + 2,0
BN2 = BN1 + BN2
BNU = (BN2/BD2)*BNU
SUM1 = BNU*BTOTAL + SUM1
800 CONTINUE
VNU1(NU+1) = VIMAG + SUM1
1000 CONTINUE
RETURN
END
SUBROUTINE COEFIF
CCCCC  CLERSH-GORDAN COEFFICIENT SUBROUTINE ( TAMURA-MARABLE - ORNL)
CCCCC  DEFINITION OF THE CG COEFFICIENT IS FOUND IN EQUATIONS
CCCCC  (16) AND (17) OF RACAH, PHYS. REV. 62 (1642) 438.
CCCCC  IF CG=(J1 J2 M1 M2 I J3 M3) THEN IA=2*J1, IB=2*J2, IC=2*J3,
CCCCC  ID=2*M1, IE=2*M2, IF=2*M3.
CCCCC  THE MAIN-ROUTINE OF A PROGRAM, ANY SUBROUTINE OF WHICH
CCCCC  IS TO CALL CLER AND/OR RAC7, MUST HAVE FOLLOWING SET
CCCCC  OF STATEMENTS AT ITS VERY BEGINNING.
C      DIMENSION FACLOG(500)
C      FACLOG(2)=FACLOG(1)=0,0
C      FN=1,0
C      DO 10 N=3,500
C      FN=FN+1,0
C  10  FACLOG(N)=LOG(FN)+FACLOG(N-1)
EQUIVALENCE (LPR,IA), (LPRPR,IB), (L,IC), (NUPR,ID), (NUPRPR,IF),
I (NU,IF)
COMMON/COEFIF/LPR,LPRPR,L,NUPR,NUPRPR,NU,COEF,RECLAMI,FACLOG(300)
105  K1=IA+IB+IC      $ IARCP=K1/2
IF(IARCP*2-K1)1000,120
120  K2=IA+ID      $ IAPD=K2/2
IF(IAPD*2-K2)1000,125
125  K3=IB+IE      $ IBME=K3/2
IF(IBME*2-K3)1000,130

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130 NZMIC2=(I8-IC-ID)/2      $ NZMIC3=(IA+IE-IC)/2
    NZMI=XMAXQF(NZMIC3,NZMIC2,0)
    NZT4=NZMI-NZMIC2      $ IABC=IABCP-IC
    NZT1=IABC-NZMI      $ IAMD=IAPD-ID
    NZT2=IAMD-NZMI      $ IBPE=IBME+IE
    NZT3=IBPE-NZMI      $ NZMX=XMINDF(IABC,IAMD,IBPE)
    IF(NZMX-NZMI)1000,2000,200
200 NZT5=NZMI-NZMIC3      $ ICPF=(IC+IF)/2      $ ICMF=ICPF-IF
    ICAB = IABCP - IB      $ IBCA = IABCP - IA
    SOFCLG = (FACLOG(IABC+1) - FACLOG(IABCP+2)
1+FACLOG(ICAB+1)+FACLOG(IBC+1)+FACLOG(IAPD+1)+FACLOG(IAMD+1)
2+FACLOG(IBPE+1)+FACLOG(IBM+1)+FACLOG(ICPF+1)+FACLOG(ICMF+1))*0,5
    TERMLG=-FACLOG(NZT1+1)-FACLOG(NZT2+1)-FACLOG(NZT3+1)
1+SOFCLG-FACLOG(NZT4+1)-FACLOG(NZT5+1)-FACLOG(NZMI+1)
    RAC=EXP(TERMLG)
    NZMI=NZMI+1
    DO 400NZ=NZMI,NZMX
    NZT3=NZT3-1      $ NZT2=NZT2-1
    NZT4=1+NZT4      $ NZT5=1+NZT5      $ NZT1=NZT1-1
    TERMLG3=FACLOG(NZT4+1)+FACLOG(NZT5+1)-FACLOG(NZ+1)
1+SOFCLG-FACLOG(NZT1+1)-FACLOG(NZT2+1)-FACLOG(NZT3+1)
    RAC=EXP(TERMLG)*RAC
400 CONTINUE
    COEF = RAC*RAC
    RETURN
2000 IF(I8)1000,2015,2010
2010 IF(=IA)200,2015,1000
1000 COEF = 0,0
    RETURN
2015 COEF = RECLAM1
    RETURN
END COEFIF
SUBROUTINE MATCNTRL
C THIS SUBROUTINE BUFFERS BLOCKS OF DATA FROM TAPE UNIT 40 CYCLICAL
C LY INTO CONSECUTIVE CELLS OF S(). IT ASSUMES LS, LSTOTAL, J, AND
C S() ARE IN COMMON. LSTOTAL IS THE DIMENSION OF S(). LS IS THE
C LENGTH OF ONE BLOCK OF S(), J IS THE INITIAL ADDRESS OF THE
C BLOCK BEING USED, OR ABOUT TO BE USED, IN THE EXTERNAL PROGRAM.
C TO USE (1) INITIATE BY SETTING J=0 AND ENTERING.
C (2) IMMEDIATELY BEFORE EACH USE OF A BLOCK OF DATA IN THE
C EXTERNAL PROGRAM PERFORM THE FOLLOWING
C J=J+LS
C IF (J-LS-1) 10, 30
C 10 IF (J+LS-1-LSTOTAL) 30, 30, 20
C 20 J=1
C 30 CALL MATCNTRL
C (3) MATCNTRL MAY BE ENTERED AT ANY OTHER POINT OF THE
C EXTERNAL PROGRAM.
C BUFFERING CONTINUES UNTIL A ONE WORD END-OF-FILE BLOCK IS READ
C IN. THE NEXT ENTRY AFTER COMPLETION OF THIS REWINDS THE TAPE.
C NO ENTRY WILL AGAIN BE EFFECTIVE UNTIL AN INITIATING ENTRY
C IS MADE WITH J = 0.
C EQUIVALENCE (INITIALS, J)
COMMON /S/ LSO, LSI, LSI*20, LS2, LS, LSTOTAL, INITIALS, S(5000)
IF (J) 19, 10
10 I=((LSTOTAL/LS)-1)*LS+1
REWIND 40
J=1
K = 0
19 IF (K) 100, 20
20 IF(UNIT, 40 )30,40,90,25
25 CALL STOP(201)
30 IF(I-J)100,20
40 I=I+LS
IF(I+LS-1-LSTOTAL)80,80,50
50 IF(I-1)70,60

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60 IF(J-1)65,100
65 J=1$GO TO E7
70 I1=1
80 IF(I1-J)85,100
85 I=I1
87 IPR=I+LS-1
  BUFFER IN( 40,1)(S(I),S(IPR))
  GO TO 20
90 REWIND 40
  K = -1
100 RETURN
  END
  SUBROUTINE MINEIG (A,V,NR,NTRY,MAXNO,EPSLON,EIGEN,S)
  DIMENSION A(2),V(2),S(2)
  MR=NR
  NRPLUS =MR+1
  NRSQ=(NRPLLS -1)*MR
  M=-1
  IF (NTRY) 7, 4, 5
5 DO 6 I = 1, MR
6 V(I) = 0,0
  NO = NTRY
  GO TO 67
7 NO = 1
  VMAX = 0,0
  DO 10 I = 1, MR
  Z = -V(I)
  IF (Z) 9, 10, 8
8 Z = -Z
9 IF (-Z-VMAX) 10, 10, 12
12 VMAX = Z
  NO = I
10 CONTINUE
  DO 11 I = 1, MR
11 V(I) = V(I)/V(NO)
  GO TO 67
  4 ANNMIN=-A(1)
  IF (ANNMIN)22,22,20
20 ANNMIN=-ANNMIN
22 NO=1
  I=NO
  DO 30 II=1,NRSQ,NRPLUS
  V(I)=0,0
  Z=-A(II)
  IF(Z)27,25,26
26 Z=-Z
27 IF(Z-ANNMIN)30,30,28
28 ANNMIN=Z
  NO=I
30 I=I+1
  GO TO 67
25 V(I)=1,0
  GO TO 28
31 Z = V(N)
  DO 32 I = 1, MR
32 V(I) = V(I)/Z
  EIGEN=(D /VMAX)*SIGN+EIGEN
33 DO 34 IJ=1,NRSQ
34 S(IJ)=A(IJ)
  DO 36 II=1,NRSQ,NRPLUS
36 S(II)=S(II)-EIGEN
  K=K+1
  IF(K)40,38
40 SIGN=-1,0
  CALL KRAMRE (S,V,MR,I,D,MR,MR)
  IF (DET) 42, 41

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41 DET = D
42 VMAX = -V(N)
   IF(VMAX)46,90,45
45 VMAX=-VMAX
   SIGN=1,0
46 T=(=0) /VMAX
   IF(T)48,38,47
47 T=-T
48 IF(=T-EPSELM )80,80,50
50 DO 60 I=1,MR
   Z=-V(I)
   IF(Z) 58,60,57
57 Z=-Z
58 IF(VMAX-Z)60,60,59
59 VMAX=Z
   N=I
60 CONTINUE
   IF(VMAX)31,65
65 DO 66 I=1,MR
66 V(I)=0,0
67 V(N0)=1,0
   K=MAXNC+1
   N=N0
   EIGEN=0,0
   DET = EIGEN
   N0=M+2
   M=N0-1
   GO TO 33
90 SIGN=0,0
   GO TO 50
80 EIGEN=(D /VMAX)*SIGN+EIGEN
38 S = DET
   MAXNC = N
   RETURN
END
SUBROUTINE DIAGONAL(X,NX,VALUE)
COMPUTES A DIAGONAL MATRIX X OF RANK NX WITH ELEMENT VALUE.
DIMENSION X(2)
N=NX
NNM=N*N-1
X(1)=VALUE
I=1
JA=1
NI=JA+N
DO 50 JB=NI,NNM,NI
X(JB+1)=VALUE
I=I+1
JI=1
JA=JA+N
DO 50 IJ=JA,JB
X(JI)=0,0
X(IJ)=X(JI)
50 JI=JI+N
RETURN
END
SUBROUTINE TRANSPOSE(X,NX)
DIMENSION X(2)
C THIS SUBROUTINE REPLACES A SQUARE MATRIX X (OF
C ORDER NX) BY ITS TRANSPOSE.
N=NX
NNM=N*N-1
I=1
JA=1
NI=JA+N
DO 50 JB=NI,NNM,NI
I=I+1

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JI=1
JA=JA+N
DO 50 IJ=JA,JB
T=X(IJ)
X(IJ)=X(JI)
X(JI)=T
JI=JI+N
50 CONTINUE
RETURN
END
SUBROUTINE MATQ (A,X,NR,NV,DET,SCALER,NA,NX)
EQUIVALENCE (SUM, SUMD), (PIVOT, PIVOTD), (Z, ZD)
DIMENSION A(2), X(2)
D = DET
K=0
KKNA=K
MX=NX
MR=NR
NRI=MR-1
KRI=NR1
NVX=(NV-1)*MX
NVXR=NVX+MR
MA=NA
NAI=MA+1
NRMRI=NAI*NRI
NRRMR=NRRRI+1
NRNAI=NRRMR-NRI
DO 5 NRNAK=NRNAI,NRRRI
PIVOT=0.0
K=K+1
NVXK=K+NVX
KKNA=KKNA+NAI
KK=KKNA-MA
DO 6 IK=KK,KRI
Z=-A(IK+1)
IF(Z) 3,6,4
4 Z=-Z
3 IF(-Z-PIVOT) 6,6,7
7 PIVOT=-Z
IPRJ=IK
6 CONTINUE
SUMD = -A(KK)
IF(SUM+PIVOT) 11,8,9
9 IF(PIVOT-SUM) 11,11,10
10 IPRJPR=IPRJ-KK+K
SUMD = -A(IPRJ + 1)
DO 12 KJ=KK,NRNAK,MA
ZD = A(IPRJ + 1)
A(IPRJ+1)=A(KJ)
A(KJ) = ZD
IPRJ=IPRJ+MA
12 CONTINUE
DO 13 KJ=K,NVXK,MX
Z=X(IPRJPR+1)
X(IPRJPR+1)=X(KJ)
X(KJ)=Z
IPRJPR=IPRJPR+MX
13 CONTINUE
D=-D
11 PIVOTD = (-1.0)/SUMD
D = -SUM*D*SCALER
DO 16 KJ=K,NVXK,MX
IJ=KJ
X(KJ)=PIVOT*X(KJ)
DO 16 IK=KK,KRI
X(IJ+1) = -A (IK+1)*X(KJ) + X(IJ+1)

```

```

IJ=IJ+1
16 CONTINUE
DO 14 KJ=KKNA, NRNAK, MA
  IJ=KJ
  A(KJ) = PIVOTD*A(KJ)
  DO 14 IK=KK, KRI
    A(IJ+1)=(-A(KJ))*A(IK+1)+A(IJ+1)
  IJ=IJ+1
14 CONTINUE
  KRI = KRI + MA
5 CONTINUE
  SUM = A(NRNR)
  IF (SUM) 17, 19
17 PIVOT = 1.0/SUM
  NRNR1 = NRNR1 + MA
  DO 18 NRJ=NR, NVXR, MX
    X(NRJ)= PIVOT*X(NRJ)
    IJ=NRJ+1
    II = NRNR1
    DO 18 K=1, NR1
      II=II-NA1
      IL=II
      IJ=IJ-1
      DO 18 LJ=IJ, NRJ
        X(IJ-1) = -A (IL+1)*X(LJ) + X(IJ-1)
      IL=IL+MA
18 CONTINUE
19 DET = D*SUM*SCALER
  RETURN
8 IF (SUM) 11, 19
  END
SUBROUTINE U VECTOR (U, V, W, N, NO, UMAX1, SCALER)
  C     HERE U IS A VECTOR OF DIMENSION NO AND SO NORMALIZED
  C     THAT THE COMPONENT U(N) OF MAXIMUM MAGNITUDE WOULD BE UNITY.
  C     HOWEVER THIS VALUE OF UNITY IS ALWAYS PROVIDED IN THE UNIT MATRIX
  C     SO THAT U(N) IS SET EQUAL TO ZERO AFTER NORMALIZATION.
  C     WE ASSUME W IS THE RESULT OF A LINEAR OPERATION, CALL IT L,
  C     OPERATING ON THE UNIT MATRIX I PLUS THE VECTOR U1 IN COLUMN N1,
  C     THE NEW VECTOR U IS DETERMINED FROM VECTOR V BY THE RELATION
  C      $L(U + I(N)) = V$  WHERE I(N) IS THE NTH COLUMN OF THE
  C     UNIT MATRIX AND V IS A GIVEN VECTOR OF DIMENSION NO.
  C     THIS SUBROUTINE REPLACES U1 BY U, N1 BY N, V AND W ARE DESTROYED,
  C     THE VALUE OF THE COMPONENT OF U OF MAXIMUM MAGNITUDE BEFORE
  C     NORMALIZATION IS PUT INTO UMAX1,
  C     MATO IS NEEDED AS A SLAVE,
  C     UMAX1 INITIALLY CONTAINS THE INITIAL SCALE FACTOR OF THE
  C     DETERMINANT GOING INTO MATO, AND SCALER IS THE CORRESPONDING
  C     MULTIPLIER SCALE FACTOR GOING INTO MATO,
  C     DIMENSION L(2), V(2), W(2)
  NU = NO
  Z = UMAX1
  CALL MATO(W, V, NU, 1, Z, SCALER, NU, NU)
  IF(Z)30,20
20 CALL STOP(301)
30 VN = 0.0
  IF(N) 25, 26
25 VN = V(N)
26 UMAX=0.0
  DO 70 I=1, NU
    U(I)=VN*U(I)+V(I)
  Z=U(1)
  IF(Z)50,70,40
40 Z=-Z
50 IF(-Z-UMAX)70,70,60
60 UMAX=-Z
  N=I

```

```

70 CONTINUE
   UMAX1 = U(N)
   UMAX = UMAX1
   IF (UMAX)90,80
80 CALL STOP(302)
90 DO 100 I=1,NU
100 U(I)=U(I)/LMAX
   U(N)=0,0 $ RETURN $ END
SUBROUTINE KRAMRD (A,X,NR,NV,DET,NA,NX)
DIMENSION A(IU),X(ID)
D=1,0
MR=NR
M=MR
KR1=M-1
NR2=KR1-1
K=0
KKNA=K
MX=NX
NX2=MX-2
NRX=NX2-NR2
NVX=(NV-1)*MX
NVXR=NVX+M
NVXM=NVXR
MA=NA
NA1=MA+1
II=NA1*NR
NRNR1=II-NA1
NRNA1=NRNR1-NR2
DO 5 NRNAK=NRNA1,NRNR1
PIVOT=0,0
K=K+1
NVXK=K+NVX
KKNA=KKNA+NA1
KK=KKNA-MA
DO 6 IK=KK,KR1
Z=-A(IK+1)
IF(Z) 3,6,4
4 Z=-Z
3 IF(-Z=PIVOT) 6,6,7
7 PIVOT=-Z
IPRJ=IK
6 CONTINUE
SUM=-A(KK)
IF(SUM+PIVOT) 11,8,9
9 IF(PIVOT-SUM) 11,11,10
10 IPRJPR=IPRJ-KK+K
SUM=-A(IPRJ+1)
DO 12 KJ=KK,NRNAK,MA
Z=A(IPRJ+1)
A(IPRJ+1)=A(KJ)
A(KJ)=Z
IPRJ=IPRJ+MA
12 CONTINUE
DO 13 KJ=K,NVXK,MX
Z=X(IPRJPR+1)
X(IPRJPR+1)=X(KJ)
X(KJ)=Z
IPRJPR=IPRJPR+MX
13 CONTINUE
D=-D
11 PIVOT=(-1,0)/SUM
DO 16 KJ=K,NVXK,MX
IJ=KJ
Z=PIVOT*X(KJ)
DO 16 IK=KK,KR1
X(IJ+1)=(A(IK+1)*Z-X(IJ+1))*SUM

```



```
85 PRODUCT = (1,E300 * A2) * (1,E300*B2)
   RETURN
80 IF (ITEST + 1998) 95, 90, 90
90 PRODUCT = A2 * B2
   RETURN
95 PRODUCT = (1,E-300*A2) * (1,E-300*B2)
   RETURN
100 PRODUCT = 0,0
    RETURN
    END
```


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