L. Lovitch and S. Rosati: THE TWO-NUCLEON SCHRODINGER EQUATION WITH TENSOR FORCES. A FORTRAN PROGRAM FOR THE $J=1^+$ BOUND AND ZERO ENERGY EIGENSOLUTION.
L. Lovitch\( ^{(x)} \) and S. Rosati: THE TWO-NUCLEON SCHRODINGER EQUATION WITH TENSOR FORCES. A FORTRAN PROGRAM FOR THE J = 1^+ BOUND AND ZERO ENERGY EIGENSOLUTIONS\(^{(+)}. \)

ABSTRACT.

A Fortran program is presented for determining the bound state and zero energy eigensolutions, and associated properties, of the neutron-proton J = 1^+ system when the interaction between the particles is described by a given combination of central, tensor and spin-orbit potentials.

1. INTRODUCTION.

The solution of the deuteron Schrödinger equation in the presence of tensor forces, that is to say, the calculation of the eigenvalue, wave functions and associated properties, in correspondence to some given potential, does not lend itself in any case to an analytic solution in closed form. A perturbation solution when the tensor force is not small is not practical, while the use of trial wave functions accompanied by a standard variational calculation of energy suffers the usual difficulties, especially when a repulsive core is present.

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The variation-iteration procedure developed by Feshbach and Schwinger\(^1\) has been used quite extensively in recent years, especially following the coding by Kalos and Blatt\(^2\) originally devised for the Illinois computer. Apart from being an indirect method, it does not always, of itself, converge rapidly and when modified accordingly results in quite extensive computations. A less essential criticism is that the latter code is written in the symbolic language of the ILLIAC and so is neither readily understood nor easily adapted for other electronic computers.

This report describes a computer program written by us in FORTRAN, which, when the neutron-proton potential is assigned, evaluates:

a) for the bound state, the eigenvalue, the associated wave functions, the percentage of the D component, the quadrupole moment and the deuteron effective range,

b) for zero energy, the corresponding wave functions, the scattering length, the effective range, and the first two shape-dependent parameters.

The method adopted, described in refs. 3) and 4), is a direct numerical integration of the equations employing middle-point matching conditions which for the zero energy case determines the solutions uniquely, while for the bound-state deuteron equations it yields a corrector formula to a trial eigenvalue giving quadratic convergence when used iteratively.

The program is composed of three subprograms. The main subprogram includes the input and output instructions and the principle calculations involved. It calls on two subprograms: the first of these is a short program which calculates the potentials at the set of net-points of the integration (allowing four possible combinations of potential shape), while the second solves the set of simultaneous linear equations that result when the continuity conditions for the inward and outward solutions are imposed at the matching-point.

2. MATHEMATICAL FORMULATION. -

Throughout, we choose 1 MeV, 1 fm and $\hbar$ as the units of energy, length and action. In terms of these the velocity of light is 197.32 MeV fm $\hbar^{-1}$, and $M$, which is twice the reduced neutron-proton mass, is 0.024114 MeV$^{-1}$fm$^{-2}$ $\hbar^2$.

The neutron-proton potential is taken to be of the form

$$V(\vec{r}) = V_C(r) + V_T(r) S_{12} + V_{LS}(r) \vec{L} \cdot \vec{S}, \quad (1)$$
where
\[ S_{12} = 3 \frac{(\vec{\sigma}_1 \cdot \vec{r})(\vec{\sigma}_2 \cdot \vec{r})}{r^2} - \vec{\sigma}_1 \cdot \vec{\sigma}_2. \]

The \( J = 1^+ \) wave function is
\[ \psi = 3 S_1 + 3 D_1 = r^{-1} \left\{ u(r) Y_{L=0, S=1}^{J=1} + w(r) Y_{L=2, S=1}^{J=1} \right\}, \tag{2} \]
where the angular momentum functions
\[ Y_{L, S}^{J} = \sum_{M_L, M_S} (LSM_L M_S / JM) Y_{L+J, M_L} (\theta, \phi) \chi_{S, M_S} \]
are proper combinations of spherical harmonics and spin functions, and in the case of the bound state, the radial functions satisfy the normalisation condition
\[ \int_0^{\infty} dr \left\{ u^2(r) + w^2(r) \right\} = 1. \tag{3} \]

The Schrödinger equation gives rise to the following coupled equations for \( u(r) \) and \( w(r) \):
\[ \frac{d^2 u}{dr^2} = \left\{ -\varepsilon + f_1(r) \right\} u + f_2(r) w, \tag{4a} \]
\[ \frac{d^2 w}{dr^2} = f_2(r) u + \left\{ -\varepsilon + \frac{b}{r^2} + f_3(r) \right\} w, \tag{4b} \]
where
\[ \varepsilon = ME, \tag{5a} \]
and
\[ f_1(r) = MV_C(r), \quad f_2(r) = 8^{1/2} MV_T(r), \tag{5b} \]
\[ f_3(r) = M \left[ V_C(r) - 2 V_T(r) - 3 V_{LS}(r) \right]. \]

The boundary conditions for the solutions are that \( u = w = 0 \) for \( r = 0 \), or at the edge of a hard core, and that \( u, w \rightarrow 0 \) as \( r \rightarrow \infty \) for the bound state, while, for the zero-energy \( \varepsilon \rightarrow 0 \) solution, the coefficient of the \( r^3 \) term in \( w \) is null, i.e. \( w_{\infty} \simeq 1/r^2 \) (we return to this later).

2.1. - The Bound state. -

For any negative value of \( \varepsilon \) (see eq. (5a)) the eqs. (4) have two linearly independent solutions \( u(\varepsilon) \) and \( w(\varepsilon) \) which are regular at the origin, and two linearly independent solutions which have the decaying asymptotic behaviour required of a bound state. From the linear combination of these an infinity of inward and outward solution can be obtained:
\[ u_{\in}(\varepsilon) = A u_{\in}^{(1)}(\varepsilon) + B u_{\in}^{(2)}(\varepsilon), \]
\[ w_{\in}(\varepsilon) = A w_{\in}^{(1)}(\varepsilon) + B w_{\in}^{(2)}(\varepsilon), \tag{6} \]
and
\[ u_{\text{out}}(\xi) = C u_{\text{out}}^{(1)}(\xi) + D u_{\text{out}}^{(2)}(\xi), \]
\[ w_{\text{out}}(\xi) = C w_{\text{out}}^{(1)}(\xi) + D w_{\text{out}}^{(2)}(\xi). \] (7)

Therefore, for a given trial energy \( \xi \), two independent solutions are integrated inward from large distances and two independent solutions are integrated outward form the origin, or edge of a hard core, until they meet at some intermediate point \( r = R \). At \( r = R \), the inward and outward solutions, and their first derivatives, can be made equal with suitable choice of \( A, B, C \) and \( D \) if and only if the trial energy value \( \xi \) coincides with an eigenvalue. In other words, an eigenvalue is given as a zero of the determinant

\[ \Delta(\xi) = \begin{vmatrix} u_{\text{in}}^{(1)}(\xi) & u_{\text{in}}^{(2)}(\xi) & u_{\text{out}}^{(1)}(\xi) & u_{\text{out}}^{(2)}(\xi) \\ w_{\text{in}}^{(1)}(\xi) & w_{\text{in}}^{(2)}(\xi) & w_{\text{out}}^{(1)}(\xi) & w_{\text{out}}^{(2)}(\xi) \\ u_{\text{in}}''(\xi) & u_{\text{in}}''(\xi) & u_{\text{out}}''(\xi) & u_{\text{out}}''(\xi) \\ w_{\text{in}}''(\xi) & w_{\text{in}}''(\xi) & w_{\text{out}}''(\xi) & w_{\text{out}}''(\xi) \end{vmatrix} \] (8)

We wish now to explain why we integrate two inward and two outward solutions rather than limit ourselves to integrating in just one direction. Let us first examine what happens if we integrate outward only. As we proceed toward the asymptotic region the general solution for \( u \) and \( w \) is of the form

\[ u \sim -A e^{-kr} + B e^{kr}, \]
\[ w \sim -C e^{-kr} \left(1 + \frac{3}{kr} + \frac{3}{k^2 r^2}\right) + D e^{kr} \left(1 - \frac{3}{kr} + \frac{3}{k^2 r^2}\right) \] (9)

The boundary conditions impose, however, that \( B \) and \( D \) be zero. But rounding off and truncation errors introduce small amounts of the unwanted solution and so sooner or later the outward solution explodes exponentially, in every case, and it is not possible to formulate a criterion which will determine the correct solution unambiguously.

To integrate inward only can be just as inaccurate, since the origin is, in general, a singular point of equs. (4). For example, if the interparticle potentials are constant around the origin, then it can be shown that the general solution for \( w \) behaves as \( 1/r^2 \) when \( r \to 0 \), while if the potentials are Yukawian then \( u \sim 1/r \) and \( w \sim 1/r^2 \) as \( r \to 0 \). It is, therefore, impossible to make \( u \) and \( w \) vanish at the origin by integrating inward.
only, since rounding off and truncation errors will always introduce part of the unwanted singular solution. Integrating both outward from the origin, or edge of a hard core, and inward from large distances, with the correct boundary conditions imposed in beginning the integrations, until they meet at some intermediate point, avoids such difficulties, since the unwanted solutions decrease in these directions, respectively.

With regard to the inward solutions, these can be started in the "extreme asymptotic" region, i.e. in the region where the nuclear potentials are zero or completely disregarded, so that the eqs. (4) result uncoupled and have the solution

\[ u(r) = N_S e^{-kr}, \]
\[ w(r) = N_D e^{-kr} \left( 1 + \frac{3}{kr} + \frac{3}{k^2 r^2} \right), \]

where \( N_S \) and \( N_D \) are constants of integration and \( k^2 = -\varepsilon \).

The range of integration can, in practice, be halved by the use of a JWKB-type approximation(3) so as to start the inward solutions of eqs. (4) in the "medium asymptotic" region, where the nuclear potentials are small but not negligible. If \( r_{j-1}, r_j \) are two successive points of the net which we consider in the numerical integration in this region, with the corresponding values \( (u_{j-1}, w_{j-1}) \) and \( (u_j, w_j) \) for the solutions of eqs. (4), then(3)

\[ \frac{u_{j-1}}{u_j} = \left[ \frac{\bar{u}_o(r_j)}{\bar{u}_o(r_{j-1})} \right]^{1/2} \exp \left[ \frac{1}{2} (r_j - r_{j-1}) \left\{ \bar{u}_o(r_j) + \bar{u}_o(r_{j-1}) \right\} \right], \]

and

\[ \frac{w_{j-1}}{w_j} = \left[ \frac{\bar{w}_o(r_j)}{\bar{w}_o(r_{j-1})} \right]^{1/2} \exp \left[ \frac{1}{2} (r_j - r_{j-1}) \left\{ \bar{w}_o(r_j) + \bar{w}_o(r_{j-1}) \right\} \right], \]

where

\[ \bar{u}_o(r) = \left[ -\varepsilon + f_1(r) + f_2(r) \frac{w(r)}{u(r)} \right]^{1/2}, \]
\[ \bar{w}_o(r) = \left[ -\varepsilon + \frac{6}{r^2} + f_3(r) \frac{u(r)}{w(r)} \right]^{1/2}. \]

The right-hand-sides of (11) then involve the ratios \( w_j/u_j \) and \( w_{j-1}/u_{j-1} \). It is sufficiently accurate in the "medium asymptotic" region to give an arbitrary value to \( w_j/u_j \) and to replace \( w_{j-1}/u_{j-1} \) in \( \bar{u}_o \) and \( \bar{w}_o \) by

\[ \frac{w_{j-1}}{u_{j-1}} = \frac{w_j}{u_j} \left( 1 + \frac{3}{kR_{j-1}} + \frac{3}{k^2 R_{j-1}^2} \right) / \left( 1 + \frac{3}{kR_j} + \frac{3}{k^2 R_j^2} \right), \]

although in principle one could iterate, i.e. insert the resulting ratios gi-
ven by (11) in (12) to obtain new values, and so on until convergence is achieved. This iteration procedure has been tested and been found to be unnecessary, giving the same final results.

As has been already observed, $\Delta(\xi)$ is zero only when $\xi$ is an eigenvalue of the system. Integrating two inward and two outward solutions for an arbitrary negative value of $\xi$ until some matching-point, $r = R$, is reached, we can choose $A$, $B$, $C$ and $D$ so that at $r = R$,

$$
\begin{align*}
  u_\text{in}(\xi) &= u_\text{out}(\xi) = u_m, \\
  w_\text{in}(\xi) &= w_\text{out}(\xi), \\
  w_\text{in}'(\xi) &= w_\text{out}'(\xi),
\end{align*}
$$

where $u_m$ is any constant value which is fixed a priori. It can be shown that if $\xi + \delta \xi$ is the exact eigenvalue then we can write a corrector formula

$$
\delta \xi = \frac{u_m \left[ u_\text{out}'(\xi) - u_\text{in}'(\xi) \right]}{\int_0^R \text{d}r \left[ u_\text{out}^2(\xi) + w_\text{out}^2(\xi) \right] + \int_\infty^R \text{d}r \left[ u_\text{in}^2(\xi) + w_\text{in}^2(\xi) \right]} + O(\delta \xi^2).
$$

Alternatively, we can choose $A$, $B$, $C$ and $D$ such that, at $r = R$,

$$
\begin{align*}
  u_\text{in}(\xi) &= u_\text{out}(\xi), \\
  u_\text{in}'(\xi) &= u_\text{out}'(\xi), \\
  w_\text{in}(\xi) &= w_\text{out}(\xi) = w_m,
\end{align*}
$$

where $w_m$ is a constant value fixed a priori; and then $\delta \xi$ is given by

$$
\delta \xi = \frac{w_m \left[ w_\text{out}'(\xi) - w_\text{in}'(\xi) \right]}{\int_0^R \text{d}r \left[ u_\text{out}^2(\xi) + w_\text{out}^2(\xi) \right] + \int_\infty^R \text{d}r \left[ u_\text{in}^2(\xi) + w_\text{in}^2(\xi) \right]} + O(\delta \xi^2).
$$

It should be noted that the use of eqs. (14) with the corrector formula (15), or eqs. (16) with the corrector formula (17) should and does yield identical results.

If, alternatively, we assume a given value for the bound state energy $\xi$, we can invert the problem, that is to say, it is possible to adjust one of the parameters of the potential so as to reproduce such an energy value. For example, if the variable parameter is a multiplicative factor which is common to the central, tensor and spin-orbit parts of the potential, so that in eqs. (4) we now have the terms $\lambda f_1$, $\lambda f_2$, $\lambda f_3$ in place of $f_1$, $f_2$ and $f_3$ respectively, then the corrector formula for this factor $\lambda$ is:
\[ \delta \lambda = \frac{-u_m \left[ u'_m(\varepsilon) - u'_m(\varepsilon) \right]}{\int_0^R \left[ u_{\text{out}} f_1^2 + w_{\text{out}}^2 f_3^2 + 2u_{\text{out}} w_{\text{out}} f_2^2 \right] + \int_0^\infty \left[ u_{\text{in}} f_1^2 + w_{\text{in}}^2 f_3^2 + 2u_{\text{in}} w_{\text{in}} f_2^2 \right]} \]

for the case that we satisfy the eqs. (14) at the matching-point \( r = R \). This corresponds to eq. (15) for \( \delta \varepsilon \). We can also readily deduce the corrector formula for \( \delta \lambda \) that may be used in conjunction with eqs. (16):

\[ \delta \lambda = \frac{-w_m \left[ w'_m(\varepsilon) - w'_m(\varepsilon) \right]}{\int_0^R \left[ u_{\text{out}} f_1^2 + w_{\text{out}}^2 f_3^2 + 2u_{\text{out}} w_{\text{out}} f_2^2 \right] + \int_0^\infty \left[ u_{\text{in}} f_1^2 + w_{\text{in}}^2 f_3^2 + 2u_{\text{in}} w_{\text{in}} f_2^2 \right]} \]

Finally, if \( \gamma^2 = -\varepsilon_d \), where \( \varepsilon_d \) is the eigenvalue of eqs. (4), then as \( r \to \infty \) we have the behaviour for the corresponding solution:

\[ u_d \sim N_d e^{-\frac{\gamma r}{2}} \text{ and } w_d \sim N_d e^{-\frac{\gamma r}{2}}. \]

The deuteron effective range is defined to be

\[ \mathcal{R}_t = \mathcal{R}(\varepsilon_d, \varepsilon_d) = \frac{1}{\gamma} - \frac{2}{N_S^2 + N_D^2}. \]

2.2. - The zero-energy solution.

Imposing the boundary conditions at the origin, or edge of a hard core, it is clear that there are two linearly independent scattering eigen solutions. These are known as the \( \alpha \)-solution and \( \beta \)-solution and are mixtures of pure \( 3S_1 \) and \( 3D_1 \) states which correspond to pure \( 3S_1 \) and \( 3D_1 \) waves respectively in the limit that the tensor force vanishes.

The general solution of eqs. (4), with \( \varepsilon = 0 \), for asymptotic values of \( r \), i.e. where the potentials vanish, is

\[ u \sim gr + h, \quad w \sim g'r^2 + \frac{h'}{r^2} \]

The \( \alpha \)-solution and \( \beta \)-solution have the properties \( g'_\alpha = 0 \) and \( h'_\beta = 0 \) respectively, and at zero and low energies the scattering occurs in the \( \alpha \)-channel. This may be described in terms of an effective range approximation for such energy values.

Consider the four linearly independent asymptotic solutions (19) of eqs. (4). We can combine these so as to obtain three linearly independent solutions possessing the property that \( g'_\beta = 0 \). Thus, to solve for the \( \alpha \)-solution we integrate two linearly independent solutions outward from the origin (or edge of hard core), with the correct zero boundary condition there, and integrate three linearly independent solutions inward from large values of \( r \), until some matching-point \( r = R \) is reached, and combine them linearly:
\[ u_{\text{out}} = A u^{(1)}_{\text{out}} + B u^{(2)}_{\text{out}}, \quad u_{\text{in}} = C u^{(1)}_{\text{in}} + D u^{(2)}_{\text{in}} + E u^{(3)}_{\text{in}}, \]
\[ w_{\text{out}} = A w^{(1)}_{\text{out}} + B w^{(2)}_{\text{out}}, \quad w_{\text{in}} = C w^{(1)}_{\text{in}} + D w^{(2)}_{\text{in}} + E w^{(3)}_{\text{in}}, \]

so that the solutions and their derivatives are continuous at \( r = R \),
\[ u_{\text{out}}(R) = u_{\text{in}}(R), \quad u'_{\text{out}}(R) = u'_{\text{in}}(R), \]
\[ w_{\text{out}}(R) = w_{\text{in}}(R), \quad w'_{\text{out}}(R) = w'_{\text{in}}(R). \]

There are therefore four equations in four unknowns, the relative mixing of the solutions (the fifth unknown may be given an arbitrary non-zero value), which have clearly a unique solution.

From the resulting solution we can derive the scattering length
\[ a_t = -\frac{h_\infty}{g_\infty} \] (20)

and the effective range
\[ r_{0t} = 2 \int_0^\infty dr \left[ (1 - \frac{r}{a_t})^2 - u_\infty^2 - w_\infty^2 \right] = \]
\[ = 2 \left[ r_f (1 - \frac{r_f}{a_t} + \frac{r_f^2}{3 a_t^2}) - \int_{r_c}^{r_f} dr \left\{ u_\infty^2 + w_\infty^2 \right\} - \frac{r_f}{3} \left\{ w_\infty (r_f) \right\}^2 \right], \] (21)

where \( r_c \) is the hard core radius, or zero if there is no hard core, and \( r_f \) is the distance from the origin of any point in the asymptotic region. It should be mentioned that the final term in expression (21) arises from evaluating directly
\[ -2 \int_{r_f}^\infty dr \, w_\infty^2. \]

The mixed effective range is given by
\[ \mathcal{G}(0, E) = 2(\mathcal{G} - \frac{1}{a_t})/\mathcal{G}^2. \] (22)

Finally, the shape parameters \( P_t \) and \( Q_t \) in the effective range approximation:
\[ k \cot \delta_\infty = -\frac{1}{a_t} + \frac{1}{2} r_{0t} k^2 - P_t r_{0t}^3 k^4 + Q_t r_{0t}^5 k^6, \] (23)

are given by(4):
\[ P_t = \left\{ 3 \left( \mathcal{Y} - \frac{1}{a_t} \right) - \mathcal{Y}^2 \left( r_{0t} + \frac{1}{2} \mathcal{Y}_t \right) \right\} / r_{0t}^3 \mathcal{Y}^4 = \]

\[ = \left\{ \frac{3}{2} \left( 0, E_d \right) - r_{0t} - \frac{1}{2} \mathcal{Y}_t \right\} / r_{0t}^3 \mathcal{Y}^2, \]

and

\[ Q_t = \left\{ -2 \left( \mathcal{Y} - \frac{1}{a_t} \right) + \frac{1}{2} \mathcal{Y}^2 \left( r_{0t} + \mathcal{Y}_t \right) \right\} / r_{0t}^5 \mathcal{Y}^6 = \]

\[ = \left\{ -\mathcal{Y} \left( 0, E_d \right) + \frac{1}{2} \left( r_{0t} + \mathcal{Y}_t \right) \right\} / r_{0t}^5 \mathcal{Y}^4. \]

If, on the other hand, we adopt the effective range approximation\(^{(7)}\) (see also eq. (3.2) of ref. \((8)\)):

\[ k \cot \alpha = - \frac{1}{a_t} + \frac{1}{2} r_{0t} k^2 + \frac{C_t}{1 + D_t r_{0t}^2 k^2}, \]  

(23a)

which may well be applicable over a larger range of values of \( k \) than eq. (23), then it may be shown that\(^{(4)}\)

\[ C_t = \frac{\left( \mathcal{Y} - \frac{1}{a_t} - \frac{1}{2} r_{0t} \mathcal{Y}^2 \right)^2}{r_{0t}^3 \mathcal{Y}^4 \left( \mathcal{Y} - \frac{1}{a_t} - \frac{1}{2} \mathcal{Y}_t \mathcal{Y}^2 \right)} = \frac{\mathcal{Y} \left( 0, E_d \right) - r_{0t}}{2 r_{0t} \mathcal{Y}^2 \left\{ \mathcal{Y} \left( 0, E_d \right) - \mathcal{Y}_t \right\}}, \]  

(24a)

and

\[ D_t = \frac{2 \left( \mathcal{Y} - \frac{1}{a_t} \right) - \frac{1}{2} \left( r_{0t} + \mathcal{Y}_t \right) \mathcal{Y}^2}{r_{0t}^2 \mathcal{Y}^2 \left( \mathcal{Y} - \frac{1}{a_t} - \frac{1}{2} \mathcal{Y}_t \mathcal{Y}^2 \right)} = \frac{2 \mathcal{Y} \left( 0, E_d \right) - r_{0t} - \mathcal{Y}_t}{r_{0t}^2 \mathcal{Y}^2 \left\{ \mathcal{Y} \left( 0, E_d \right) - \mathcal{Y}_t \right\}}. \]  

(25a)

3. PROGRAM DESCRIPTION.

The program was originally written in FORTRAN II, but at an intermediate stage of the testing it was decided to translate it to FORTRAN IV (due to changes in the computer facilities available to us). We therefore present the FORTRAN IV version of the program, and keeping in mind the fact that FORTRAN II is still being used extensively, we note that the only changes required to obtain a FORTRAN II version are appropriate modifications in the input and output statements and to the names, in call statements, of the subprograms of the system.

The program listing that we present yields double precision operations for all floating-point calculations. To obtain double precision results it is not necessary to perform all these calculations in double precision, but it was felt that the greater simplicity resulting, combined with the
very small time difference involved on an IBM 7094 computer, justified our doing so. To change to single precision calculations, all that is then needed is to replace the D-conversion by E-conversion for the floating point constants and in format statements associated with the input and output, and to remove all type statements "Double Precision . . . ." that appear towards the beginning of each subroutine.

The entire program consists of a main routine and two subroutines. The main routine executes the bulk of the calculations and the input and output instructions, subroutine POT calculates the potential functions normalised accordingly, and subroutine SYSTEM performs the solution of a set of simultaneous linear equations of arbitrary order (we need to solve a set of three equations prior to evaluating the corrector formula for the bound state, and a set of four equations to match the zero-energy scattering solutions).

We present the listing of the main program and subroutine POT in Appendix A. For subroutine SYSTEM (A, N, B) any standard subprogram that solves the set of N simultaneous linear equations, which we write in matrix form

\[ AX = B, \quad (26) \]

and which, before returning execution to the calling program, replaces the array B by the solution X of the system, may be used. The subprogram used by us was based on a program MATINV existing in the SHARE catalogue available to users of IBM machines. For compatibility with the main program it is necessary that A and B of subroutine SYSTEM be dimensioned as A(4,4) and B(4) respectively.

Subroutine POT yields the central, tensor and spin-orbit potentials at the set of net-points of the integration range combined, and normalised, in a form suitable for direct insertion in the differential equations. The well shapes of the potentials calculated may be

Square well : \[ V(r) = \begin{cases} V_0, & r < r_0, \\ 0, & r > r_0 \end{cases}, \]

Exponential well : \[ V(r) = V_0 e^{-\mu r}, \]

Yukawa well : \[ V(r) = \frac{V_0 e^{-\mu r}}{\mu r}, \]

Gauss well : \[ V(r) = V_0 e^{-\alpha r^2}. \]

and there may or may not be a hard core associated with the two-particle interaction. The information necessary to define the potentials is transmitted to the subroutine from the main program, after being specified by the input data.
3.1. - Main Subprogram. -

The most important part of this program for the causal user consists of the input statements, so that once a set of input data is specified the machine effects the calculations requested by the data. There are three such input statements: they are preceded by the external formula numbers 2, 4 and 6 and are associated respectively with the format statements having external formula numbers 500, 504 and 516.

Since, in general, the nuclear potentials are short ranged and vary strongly near the origin, it is necessary, when solving the differential equations, to use small integration step-lengths in this region; while on the other hand, when we reach a region where the potentials become small, it may be sufficient to use much larger step-lengths to obtain a particular accuracy and, indeed, it would be extremely wasteful of machine-time to use the same step-length over the whole range of integration besides requiring a corresponding increase in the capacity of the memory of the computer. We have therefore allowed for the possibility of using different integration step-lengths, dividing up the total range of integration of the equations into blocks, each of which is subdivided into a certain number of intervals of equal length. Clearly, the actual step-lengths to be used for a particular problem depends essentially on the accuracy desired for the results; nevertheless we feel it worthwhile stating, as an illustration, that, to obtain very accurate results with some potentials, step-lengths of about 0.001 fm had to be used near the origin, whereas at about 2 fm away from it step-lengths of 0.2 fm were already quite adequate.

The first input statement:

\[ 2 \text{ READ}(5,500) \text{ CORE}, H(1), J\Theta T, (N(L),X(L),L=1,J\Theta T) \]

associates the numbers on the first few data cards with respectively, the hard core radius, the step-length to be used nearest the origin, the number of blocks to be used in the outward integration, the total number of blocks to be used over the entire integration range, followed by the number of step-lengths to be used in the first block (i.e. the one nearest the origin), the step-length scale factor in going from the first to second block, the number of step-lengths to be used in the second block, the step-length scale factor in going from the second to the third integration block, and so on until the number of step-lengths in the final block is read.

The machine then proceeds to calculate the distance from the origin of each of the integration net-points and the appropriate factors that should be associated with them in the numerical integration of simple quadratures, such as is required later to normalise the wave functions. The numerical integration formula used for these quadratures is the three-point SIMPSON rule.

In the second input statement of the program:

\[ 4 \text{ READ}(5,504) \text{ IV, VC, RC, VT, RT, VL, RL} \]

the first quantity is the one which decides whether square wells, exponential-
tials wells, Yukawa wells or Gauss wells are to be used for the central, tensor and spin-orbit potentials of the nuclear force interaction. This is followed successively by the depth and range of each of these three potentials. The depths should in all cases be presented in MeV, positive for a repulsive potential and negative for an attractive potential, whereas the ranges for a square well, exponential well, Yukawa well, Gauss well should be given in fm, fm$^{-1}$, fm$^{-1}$, fm$^{-2}$ respectively. It should be noted that if a calculation is to be made with a neutron-proton potential having no spin-orbit term and using Yukawa potentials for the central and tensor parts, then a non-zero value should be assigned to the range of the spin-orbit term.

The third and final input statement of the program:

reads a trial energy for the bound state (this should be negative), and the minimum significance to be accorded to the successive corrections to the energy value in MeV. Thus, if a correction is less than the latter quantity in absolute value (it may be given as zero), then the energy search is terminated. As has been already mentioned, however, the accuracy is limited rather by the step-lengths used in the integration formula. Therefore, if we require a value of the energy accurate to 0.001 MeV for the potentials of Appendix B, say, then we may obtain such an accuracy with single precision calculations dividing the range of integration into step-lengths of 0.01 fm for $0 < r < 0.2$, 0.02 fm for $0.2 < r < 0.8$, 0.04 fm for $0.8 < r < 2.0$ and 0.4 fm for $2.0 < r < 12.0$. Putting the next number (IC) equal to 1, 2 or 3 instructs the machine to calculate the solution to the bound state problem only, the solutions to the bound state and scattering at zero energy, or the zero-energy scattering solution only respectively. The succeeding numbers stipulate the re-entry point at the end of a given calculation; which wave functions (if any) are desired in the output; whether, in solving the bound state problem, we wish to use eqs. (14) and (15) or eqs. (16) and (17) (we have already pointed out that these will give the same final results); whether to use the "extreme asymptotic" solution given by eqs. (10) or the JWKB solution of eqs. (11), (12) and (13) for starting the inward integrations, in the case of the bound state problem; and, finally, the maximum number of iterations to be used in solving the bound state problem.

With regard to the re-entry point, we have allowed for a re-entry at any one of the three input statements. Hence, for example, if we wish to change the potential without altering the net-points over the range of the integration we can make the re-entry at the second input statement. For starting the inward integrations in the case of the bound state problem, clearly the "extreme asymptotic" solution is the more indicated for square-well potentials since these are exactly zero further than a certain distance from the origin. In all other cases, the JWKB solution makes it possible to reduce the total range of integration by about a factor of two as compared with the "extreme asymptotic" solution, in obtaining the same accuracy. For example, to obtain more than five figure accuracy for the energy...
of a bound state, it is necessary to integrate inward from about 27 fm if we use the "extreme asymptotic" solution, whereas with the JWKB solution somewhere between 12 and 17 fm suffices for this purpose. To conclude our comments on the input statements we should mention that we have found that the solution to the bound state problem generally converges in between three and five iterations. All further details regarding the input statements are contained in comments at the beginning of the subprograms, listing of which are given in Appendix A. In Appendix B we give a sample set of input data, while in Appendix C we give a sample set of results obtained using the first set of data listed in Appendix B.

In conclusion, we feel that some comments on the numerical integration of the differential equations are appropriate. In the program, we have used the NUMEROV recurrence relation(6) to integrate inside each of the blocks into which the range of integration is divided, and a generalisation of it(3) to continue the solution from one block of a given step-length size to another one.

If we write eqs. (4) in matrix form

$$\frac{d^2Y}{dr^2} = V(r)Y,$$  \hspace{1cm} (28)

then, if h is the step-length in a given block, writing

$$Z = Y - \frac{1}{12}h^2Y^{(2)},$$ \hspace{1cm} (29)

where \(Y^{(2)}\) is the second derivative of \(Y\) with respect to \(r\), the NUMEROV recurrence relation is

$$Z_{n+1} = 2Z_n - Z_{n-1} + h^2Y^{(2)}_n = 12Y_n - 10Z_n - Z_{n-1},$$ \hspace{1cm} (30)

with an error of approximately \(-\left(h^6/240\right)Y^{(6)}_n\).

To continue the solution from one block of step-lengths to the next let \(Y_n, Y_{n+k}, Y_{n-1}\) be, respectively, the values of \(Y\) at \(r_n, r_{n+k}, r_{n-1}\) for arbitrary values of \(k\) and \(l\), then

$$1\left[Y_{n+k} - \frac{1}{12}h^2(k^2 + kl - l^2)Y^{(2)}_{n+k}\right] = (1+k)\left[Y_n + \frac{1}{12}h^2(l^2 + 3lk + k^2)Y^{(2)}_n\right] - k\left[Y_{n-1} - \frac{1}{12}h^2(l^2 + lk - k^2)Y^{(2)}_{n-1}\right],$$ \hspace{1cm} (31)

with an error \(O(h^5)\) when \(k \neq 1\), and which reduces to eq. (30) when \(k = 1\).

These are the most accurate three-point formulas that may be used to integrate eqs. (29). More accurate integration formulae involving a larger number of points can be derived, such as for example, the predictor-corrector formulae of Milne

$$Y_{n+1} = Y_n + Y_{n-1} - Y_{n-3} + \frac{h^2}{4}(5Y^{(2)}_n + 2Y^{(2)}_{n-1} + 5Y^{(2)}_{n-2}) + O(h^6),$$ \hspace{1cm} (32)

$$Y_n = 2Y_{n-1} - Y_{n-2} + \frac{h^2}{12}(Y^{(2)}_n + 10Y^{(2)}_{n-1} + Y^{(2)}_{n-2}) + O(h^6),$$
14.

over five points. The use of more accurate formulae would permit one to use larger integration step-lengths and though they involve a larger number of elementary operations there would probably be a net reduction in the calculation time. More important still is the saving in the memory store of the computer which could be extremely important in the inverse problem of searching for a potential, of a given type, to fit the deuteron data and scattering phase shifts over a range of energy values.

REFERENCES. -

(1) - H. Feshbach and J. Schwinger, Phys. Rev. 84, 194 (1951).
(2) - M. H. Kalos and J. M. Blatt, Univ. of Illinois, Digital Computer Laboratory, Internal report n. 50 (1953, unpublished).
(4) - L. Lovitch and S. Rosati, preprint.
DIRECT NUMERICAL SOLUTION, WITH MIDDLE-POINT MATCHING, OF
THE DEUTERON EQUATIONS WITH TENSOR FORCES GIVING THE ENERGY
EIGENVALUE, PERCENTAGE D-STATE AND QUADRUPOLE MOMENT, AND/OR
THE SCATTERING LENGTH AND EFFECTIVE RANGE TOGETHER WITH THE
ASSOCIATED WAVE FUNCTIONS.

VARIOUS STEP-LENGTHS CAN BE USED IN INTEGRATING OVER THE
TOTAL RANGE.

JTOT = TOTAL NUMBER OF BLOCKS OF DIFFERENT STEP-LENGTHS
JOUT = NUMBER OF BLOCKS USED IN INTEGRATING OUTWARD
RMAX = RANGE OF INTEGRATION FOR LAST ITERATION IN SEARCHING FOR
THE EIGENVALUE, OR WHEN CALCULATING THE SCATTERING LENGTH AND
EFFECTIVE RANGE.
N(L) = NUMBER OF STEP-LENGTHS IN L-TH BLOCK
X(L) = STEP-LENGTH SCALE FACTOR IN GOING FROM L-TH TO (L+1)-TH
BLOCK.

CORE = HARD CORE RADIUS OF POTENTIAL
VC, RC, VT, RT, VL, RL ARE THE PARAMETERS OF POTENTIAL
AND IV DEFINES ITS TYPE - CF. SUBPROGRAM POT FOR FURTHER DETAILS

E0 = TRIAL ENERGY VALUE FOR EIGENVALUE PROBLEM - NEGATIVE
EPS IS ACCURACY REQUIRED FOR EIGENVALUE - THIS CAN BE ZERO
IC = 1 FOR SOLVING THE EIGENPROBLEM ONLY
IC = 2 FOR SOLVING THE EIGENVALUE PROBLEM AND SCATTERING LENGTH
AND EFFECTIVE RANGE.
IC = 3 FOR EVALUATING THE SCATTERING LENGTH AND EFFECTIVE RANGE.
IPR = 1 TO PRINT U1, W1, U2, W2, U, W AT END OF FINAL ITERATION
IPR = 2 TO PRINT U, W AT END OF FINAL ITERATION
IPR = 3 TO PRINT U1, W1, U2, W2, U, W DURING EACH ITERATION
IPR = 4 TO PRINT U, W DURING EACH ITERATION
IPR = 5 FOR NO SOLUTION PRINT-OUT
M = 1, 2, 3 GIVES REENTRY AT Z, 4, 6 RESPECTIVELY
IC = 1 FOR MATCHING EXACTLY U, W RESPECTIVELY AND, IN CASE OF
EIGENVALUE PROBLEM, THE CORRECTOR FORMULA IS GIVEN IN TERMS OF
THE MISMATCH OF W, U RESPECTIVELY.
KCH = 1, 2 FOR EXTREME ASYMPOTIC, JWB SOLUTION RESPECTIVELY
FOR INITIATING THE INWARD SOLUTION.
RS1, RS2 ARE INITIAL RATIOS OF THE TWO INDEPENDENT D-WAVE/S-WAVE
SOLUTIONS AT THE FIRST STEP LENGTH FROM THE HARD CORE RADIUS
RF1, RF2 ARE INITIAL RATIOS OF THE TWO INDEPENDENT D-WAVE/S-WAVE
SOLUTIONS AT THE FIRST STEP-LENGTH FROM THE END OF INTEGRATION
RANGE.
G1, G2 ARE THE VALUES OF G FOR THE ZERO-ENERGY ASYMPTOTIC
ALPHA S-WAVE SOLUTIONS, 1 + G*H

DIMENSION N(10)
DIMENSION H(10), A(4), W(10), R(300), S(300), U(1300), U2(300),
1 U(300), W(300), W(300), U(300), W(300), W(300)
2 F2(300), F3(300), U2S(300), W2S(300), U3(300), W3(300)
COMMON HTM , RAD2 , RAD3
DOUBLE PRECISION Q , RHOT , SCL , ROT , ASDP
DOUBLE PRECISION SOP , VC , RC , VT , RT
DOUBLE PRECISION VR , RL , EPS , CL , C2
DOUBLE PRECISION H , HV , K , SIMP , U1
DOUBLE PRECISION U2 , U , W1 , W2 , W
DOUBLE PRECISION K , A , X , P1 , P2
DOUBLE PRECISION F3 , U2S , W2S , U3 , W3
DOUBLE PRECISION HTM , RAD2 , DSQR , RAD3 , H1
DOUBLE PRECISION CORE , RM , DE , EE , E0
DOUBLE PRECISION P , P1 , P2 , P3 , P4
DOUBLE PRECISION ER , G1 , G2 , G3 , RF1
DOUBLE PRECISION RF2 , C , CL , C2 , A1
DOUBLE PRECISION B1 , DEXP , XM , S31 , Z31
DOUBLE PRECISION Z32 , Z32 , S11 , Z11 , S21
DOUBLE PRECISION Z21 , S12 , Z12 , S22 , Z22
DOUBLE PRECISION Z13 , S23 , Z23 , S33
DOUBLE PRECISION Z33 , C3 , AZ , BE , U1OUT
DOUBLE PRECISION W1OUT , U2OUT , W2OUT , DFLOAT , DUOUT
DOUBLE PRECISION DUOUT , DW1OUT , DW2OUT , U3IN , W3IN
DOUBLE PRECISION DU3IN , DW3IN , U1IN , W1IN , U2IN
DOUBLE PRECISION W2IN , UIK2 , U2K2 , WIK2 , W2K2
DOUBLE PRECISION DU3IN , DU3IN , DW3IN , W2IN , R31
DOUBLE PRECISION RS2 , WM , UM , F , PD
DOUBLE PRECISION SS5 , AMFR

500 FORMAT(2D10.5,215/5(15,D10.5))
504 FORMAT(I5*6,D12.6)
508 FORMAT(I1H,35X,43H SOLUTION OF SCHROEDINGER DEUTERON EQUATION
1/ 2STH INITIAL PARAMETER VALUES
2L STEP LENGTH 7X17H NUMBER OF BLOCKS/D219**521**3X122] /// 44H
3INWARD INTEGRATION - NUMBER OF BLOCKS JOUT= 13 // 4(13H N H X
4X 1/(4(15*2D11*4*4*4))
510 FORMAT(// 26H MATCHING POINT ABCISSA =D12.4 /// 43H INWARD INTEGRATION - NUMEP OF BLOCKS JIN= 13 // 4(13H N H X
2 1/(4(15*2D11*4*4*4))
512 FORMAT(/// 32H PARAMETERS SPECIFYING POTENTIAL ///
1 5H IC3X=8H M KCH5X=3H G1 12X=3H G2 12X=3H G3 12X=4H RF1
2 3H WL 12X=3H RL /110X3X60156)
516 FORMAT(2D10.6,6I5)
520 FORMAT(/// 35H REMAINING DATA SPECIFYING SOLUTION ///
1 5H IC3X=8H M KCH5X=3H G1 12X=3H G2 12X=3H G3 12X=4H RF1
2 11H4H RF2 11H4H RS1 11H4H RS2 /31570156)
522 FORMAT(1H1)
524 FORMAT(5X,3I1H UNRENORMALISED S-WAVE SOLUTION //6(2I1H R(L)
1U1(L))
528 FORMAT(1H15X,3I1H UNRENORMALISED S-WAVE SOLUTION //6(2I1H R(L)
1U2(L))
530 FORMAT(1H15X,3I1H UNRENORMALISED S-WAVE SOLUTION //6(2I1H R(L)
1U3(L))
532 FORMAT(1H15X,3I1H UNRENORMALISED D-WAVE SOLUTION //6(2I1H R(L)
1W1(L))
536 FORMAT(1H15X,3I1H UNRENORMALISED D-WAVE SOLUTION //6(2I1H R(L)
1W2(L))
538 FORMAT(1H15X,3I1H UNRENORMALISED D-WAVE SOLUTION //6(2I1H R(L)
1W3(L))
540 FORMAT(6(1PD 9.2, D12.5))
544 FORMAT(/// 4H IT= 13, 4H EO= 1PD15.7, 4H EE= D15.7, 4H DE=
1D15.7X18H B(1/3) = 3D15.7)
548 FORMAT(1H18X=25H DEUTERON S-WAVE SOLUTION / 6(2I1H R(L)
1(L))
552 FORMAT(1H18X=25H DEUTERON D-WAVE SOLUTION / 6(2I1H R(L)
1(L))
556 FORMAT(///20X=4H EO= 1PD15.7X3X3H 0OPD15.7X3X4H PD=1PD15.7/)\n560 FORMAT(/// 35X=18H SCATTERING LENGTH 10X=16H EFFECTIVE RANGE /
1 D48.6D26.6/)
562 FORMAT(///20X=18H SCATTERING LENGTH 10X=16H EFFECTIVE RANGE 10X,
116H SHAPE PARAMETER /1PD36*6D27*6OPD26*6/3X22H MIXED EFFECTIVE
2X 3X DEUTERON EFFECTIVE RANGE 3X=26H APPROX. SHAPE PARAMETER
3ER 3X, 23H SECOND SHAPE PARAMETER /1PD17*6D28*6OPD29*6D26*6/)
564 FORMAT(///56H TRIAL ENERGY HAS GONE POSITIVE+ CALCULATION INTERRUPT
1ED)

C
EQUIVALENCE (U1,U),(W1,W),(U2,U2),(W2,W2)

C
HTM=0.024114300
RAD2=DSQRT(2.*DO)
RAD3=DSQRT(3.*DO)

C
READ (5,500) CORE,H(1),JOUT,JTOT,(N(L),X(L),L=1,JTOT)

C
JIN=JTOT-JOUT
XIJTOT=1.00
XIJOUT=1.00

Hlv::H

DO 3 L=1,JTOT
H(L)=H(L)
HV(L)=HI*H1/12.00
HI=H1*X(L)

3
C
INTEGRATION COEFFICIENTS

17
K=0
K1=1
R=CORE+H
SIMP=6.00*H/3.00

DO 65 L=1,JTOT
HI=H(L)
K2=N(L)

IF(L-1)=41,41,29
IF(L-JOUT-1)=37,33,37

NT2=K1
NT3=K
NT4=K-1

RM=R(K)

A=H1/3.00
SIMP(K)=SIMP(K)+A
SIMP(K1)=6.00*A
R(K1)=R(K)+H1

41
DO 45 IB=2,K2

K=K1
K1=K+1
R(K1)=R(K)+H1

45
SIMP(K1)=H1+H1-SIMP(K)

49
IF(SIMP(K1)-H1)=53,57,57

53
SIMP(K1)=0.500*SIMP(K1)

GO TO 61

57
SIMP(K1)=0.37500*SIMP(K1)
SIMP(K)=1.25000*SIMP(K)

61
K=K1
K1=K+1
NT=K
NT1=NT-1
HI=1.00/H(JOUT)

C
READ (5,504)IV,VC,RC,VT,RT,VL,RL

C
CALL POT(IV,VC,VT,VL,RC,RT,RL,JTOT,JOUT,N,H,X,HV,R,F1,F2,F3)

DE=0.00

C
READ (5,516)E0,EPS,IC,IR,IPR,M,KCH,MAXIT
RS1=2.50000
RS2=5.00000
RF1=7.00-D-2
RF2=1.00-D-2
G1=-1.00
G2=-0.500
G3=0.100

C
WRITE (6,522)
WRITE (6,508)CORE,H(1),JTOT,JOUT,(N(L),H(L),X(L),L=1,JOUT)
  L=JOUT+1
C
WRITE (6,510)RM,JIN,(N(L),H(L),X(L),L=L1,JTOT)
WRITE (6,512)IV, VC, RC, VT, RT, VL, RL
WRITE (6,520)IC,M,KCH,G1,G2,G3,RF1,RF2,RS1,RS2
WRITE (6,522)
C
GO TO (69,73,73),IC
69
IC=IC
GO TO 77
73
IC=IC=1
C
GO TO (81,85),IC
81
EE=HTM*EO
GO TO 87
85
EO=O.DO
EE=EO
87
DE=EE+DE
C
GO TO (97,107),IC
93
DO 373 IT=1*MAXIT
97
P=DSQRT(-EE)
C
P1-P4 ARE CORRECTIONS FOR THE FINAL INTEGRATION COEFFICIENT
SIMP(NT) TO TAKE INTO ACCOUNT TAIL OF WAVE FUNCTION
C
P1=0.5DO/P
A=1.DO/(P*PI(NT))
B=1.DO/(1.DO+3.DO*A*(1.DO+A))
P2=P1*B*B*(1.DO+6.DO*A*(1.DO+A*(2.DO+A)))
P3=P1*B*B*(1.DO+A*(4.DO+5.DO*A))
P4=P1*B*B*(1.DO+A*(7.DO+A*(18.DO+18.DO*A)))
K=0
C
DO 117 L=1,JTOT
ER=DE*HV(L)
L1=N(L)-1
DO 110 IB=1,L1
K=K+1
F1(K)=F1(K)-ER
F3(K)=F3(K)-ER
IF(L-JOUT) 112,111,111
ER=ER*X(L)*X(L)
112
K=K+1
F1(K)=F1(K)-ER
F3(K)=F3(K)-ER
C
A=RI(NT)
B=RI(NT1)
C
GO TO (126,125),IC
C
BOUNDARY VALUES OF ZERO ENERGY FUNCTIONS
C
DO 125 U1(NT)=1.DO+A*G1
U2(NT)=1.DO+A*G2
U3(NT)=U1(NT)
W1(NT)=1.DO/(A*A)
W2(NT)=W1(NT)
W3(NT)=G3*W1(NT)
U1(NT1)=1*D0+B*G1
U2(NT1)=1*D0+B*G2
U3(NT1)=U1(NT1)
W1(NT1)=1*D0/(B*B)
W2(NT1)=W1(NT1)
W3(NT1)=G3*W1(NT1)
GO TO 131

C
C BOUNDARY VALUES OF FUNCTIONS

126 U1(NT)=1*D-10
U2(NT)=1*D-10
W1(NT)=U1(NT)*RF1
W2(NT)=U2(NT)*RF2
C=A/B
C1=P*A
C2=P*B
C=C*(C2*(C2+3*D0)+3*D0)/(C1*(C1+3*D0)+3*D0)
C1=RF1*C
C2=RF2*C

C
GO TO (127,128),KCH

127 A1=DEXP((P*HIJTOT))
U1(NT1)=U1(NT)*A1
U2(NT1)=U2(NT)*A1
W1(NT1)=W1(NT)*A1*C
W2(NT1)=W2(NT)*A1*C
GO TO 131

C
C JWKB APPROXIMATION

128 A1=DSQRT(F1(NT)+F2(NT)*RF1)
A1(2)=DSQRT(F1(NT)+F2(NT)*RF2)
A1(3)=DSQRT(F3(NT)+F2(NT)/RF1)
A1(4)=DSQRT(F3(NT)+F2(NT)/RF2)
B1=DSQRT(F1(NT1)+F2(NT1)*C1)
U1(NT1)=U1(NT)*DEXP((A1+B1)* RAD3 )*DSQRT(A1/B1)

C
B1=DSQRT(F1(NT1)+F2(NT1)*C2)
U2(NT1)=U2(NT)*DEXP((A1(2)+B1)* RAD3 )*DSQRT(A1(2)/B1)

C
B1=DSQRT(F3(NT1)+F2(NT1)/C1)
W1(NT1)=W1(NT)*DEXP((A1(3)+B1)* RAD3 )*DSQRT(A1(3)/B1)

C
B1=DSQRT(F3(NT1)+F2(NT1)/C2)
W2(NT1)=W2(NT)*DEXP((A1(4)+B1)* RAD3 )*DSQRT(A1(4)/B1)

C
C START INWARD INTEGRATION

131 K=NT
K1=NT1
L1=JIN
L2=-1

C
135 ICL=ICC+L2-1
DO 187 L=1,L1
139 IF(L2)143,143,147
143 JR=JTOT-L+1
XM=1.DO/(X(JR)*X(JR))
IF( ICL ) 163, 145, 163

145 S31=(1.DO-F1(K)*XM)*U3(K)-F2(K)*XM*W3(K)
Z31=(1.DO-F3(K)*XM)*W3(K)-F2(K)*XM*U3(K)
S32=(1.DO-F1(K))*U3(K)-F2(K)*W3(K)
Z32=(1.DO-F3(K))*W3(K)-F2(K)*U3(K)
GO TO 163

C 147 JR=L
151 IF(L-1) 155, 159
155 S11=0.DO
Z11=0.DO
S21=0.DO
Z21=0.DO
GO TO 167
159 XM=X(L-1)**2

C S AND Z ARE AUXILIARY VARIABLES FOR THE SOLUTIONS
C

163 S11=(1.DO-F1(K)*XM)*U1(K)-F2(K)*XM*W1(K)
Z11=(1.DO-F3(K)*XM)*W1(K)-F2(K)*XM*U1(K)
S21=(1.DO-F1(K)*XM)*U2(K)-F2(K)*XM*W2(K)
Z21=(1.DO-F3(K)*XM)*W2(K)-F2(K)*XM*U2(K)

C 167 S12=(1.DO-F1(K1))*U1(K1)-F2(K1)*W1(K1)
Z12=(1.DO-F3(K1))*W1(K1)-F2(K1)*U1(K1)
S22=(1.DO-F1(K1))*U2(K1)-F2(K1)*W2(K1)
Z22=(1.DO-F3(K1))*W2(K1)-F2(K1)*U2(K1)

C K=K+L2
K1=K1+L2
K2=N(JR)

C 171 DO 175 IB=2*K2
S13=10.DO*U1(K)-S12+U1(K1)+(U1(K)-S11)
Z13=10.DO*(W1(K)-Z12)+W1(K1)+(W1(K)-Z11)
S23=10.DO*U2(K)-S22+U2(K1)+(U2(K)-S21)
Z23=10.DO*(W2(K)-Z22)+W2(K1)+(W2(K)-Z21)

C A=1.DO/((1.DO-F1(K1))*(1.DO-F3(K1))-F2(K1)*F2(K1))
U1(K1)=A*(Z13*F2(K1)+S13*(1.DO-F3(K1)))
W1(K1)=A*(Z13*(1.DO-F1(K1))+S13*F2(K1))
U2(K1)=A*(Z23*F2(K1)+S23*(1.DO-F3(K1)))
W2(K1)=A*(Z23*(1.DO-F1(K1))+S23*F2(K1))

C IF( ICL ) 174, 173, 174

173 S33=10.DO*U3(K)-S32+U3(K1)+(U3(K)-S31)
Z33=10.DO*(W3(K)-Z32)+W3(K1)+(W3(K)-Z31)
U3(K1)=A*(Z33*F2(K1)+S33*(1.DO-F3(K1)))
W3(K1)=A*(Z33*(1.DO-F1(K1))+S33*F2(K1))
S31=S32
S32=S33
Z31=Z32
Z32=Z33
S11=S12
S12=S13
Z11=Z12
Z12=Z13
S21=S22
\[
\begin{align*}
S22 &= S23 \\
Z21 &= Z22 \\
Z22 &= Z23 \\
K &= K + L2 \\
K1 &= K1 + L2
\end{align*}
\]

CONTINUING THE SOLUTIONS FROM ONE STEP-LENGTH TO THE NEXT

\[
\begin{align*}
\text{IF} (L2) & \text{179.179.181} \\
\text{IF} (L1) & \text{187.187.187}
\end{align*}
\]

\[
\begin{align*}
B &= 1 + D0 + A^2 (1 + D0 - A) \\
A &= 1 + D0 + A^2 \\
C &= 1 + D0 + A^2 (3 + D0 + A) \\
K2 &= K - L2
\end{align*}
\]

\[
\begin{align*}
A1 &= 1 + D0 - B * F1(K1) \\
B1 &= B * F2(K1) \\
A2 &= B1 \\
B2 &= 1 + D0 - B * F3(K1) \\
B &= 1 + D0 / (A1 * B2 - B1 * A2)
\end{align*}
\]

\[
\begin{align*}
C1 &= (1 + D0 + A) * (U1(K) + B * C * (U1(K) - S12)) - A * (U1(K2) - C3 * (U1(K2) - S11)) \\
C2 &= (1 + D0 + A) * (W1(K) + C * (W1(K) - Z12)) - A * (W1(K2) - C3 * (W1(K2) - Z11)) \\
U1(K1) &= (C1 * B2 - C2 * B1) * B \\
W1(K1) &= (C2 * A1 - C1 * A2) * B
\end{align*}
\]

\[
\begin{align*}
C1 &= (1 + D0 + A) * (U2(K) + B * C * (U2(K) - S22)) - A * (U2(K2) - C3 * (U2(K2) - S21)) \\
C2 &= (1 + D0 + A) * (W2(K) + C * (W2(K) - Z22)) - A * (W2(K2) - C3 * (W2(K2) - Z21)) \\
U2(K1) &= (C1 * B2 - C2 * B1) * B \\
W2(K1) &= (C2 * A1 - C1 * A2) * B
\end{align*}
\]

\[
\begin{align*}
\text{IF} (L1) & \text{187.185.187} \\
C1 &= (1 + D0 + A) * (U3(K) + B * C * (U3(K) - S32)) - A * (U3(K2) - C3 * (U3(K2) - S31)) \\
C2 &= (1 + D0 + A) * (W3(K) + C * (W3(K) - Z32)) - A * (W3(K2) - C3 * (W3(K2) - Z31)) \\
U3(K1) &= (C1 * B2 - C2 * B1) * B \\
W3(K1) &= (C2 * A1 - C1 * A2) * B
\end{align*}
\]

\[
\begin{align*}
U1OUT &= U1(K) \\
W1OUT &= W1(K) \\
U2OUT &= U2(K) \\
W2OUT &= W2(K)
\end{align*}
\]

\[
\begin{align*}
S13 &= (1 + D0 - F1(K1)) * U1(K1) - F2(K1) * W1(K1) \\
S23 &= (1 + D0 - F1(K1)) * U2(K1) - F2(K1) * W2(K1) \\
Z13 &= (1 + D0 - F3(K1)) * W1(K1) - F2(K1) * U1(K1) \\
Z23 &= (1 + D0 - F3(K1)) * W2(K1) - F2(K1) * U2(K1)
\end{align*}
\]

\[
\begin{align*}
A &= L2
\end{align*}
\]

\[
\begin{align*}
\text{DU1OUT} &= A * ((S11 - S13) + 0.5D0 * (U1(K1) - U1(K2))) \\
\text{DU2OUT} &= A * ((S21 - S23) + 0.5D0 * (U2(K1) - U2(K2))) \\
\text{DW1OUT} &= A * ((Z11 - Z13) + 0.5D0 * (W1(K1) - W1(K2))) \\
\text{DW2OUT} &= A * ((Z21 - Z23) + 0.5D0 * (W2(K1) - W2(K2)))
\end{align*}
\]

\[
\begin{align*}
\text{IF} (L1) & \text{189.188.189} \\
U3IN &= U3(K) \\
W3IN &= W3(K) \\
S33 &= (1 + D0 - F1(K1)) * U3(K1) - F2(K1) * W3(K1)
\end{align*}
\]
Z33 = (1*D0 - F3(K1)) * W3(K1) - F2(K1) * U3(K1)
DU3IN = ((S31 - S33) + 0.5*D0 *(U3(K1) - U3(K2))) * H1
DW3IN = ((Z31 - Z33) + 0.5*D0 *(W3(K1) - W3(K2))) * H1

C

189 IF(L2) 193, 193, 197

193 U1IN = U1OUT
W1IN = W1OUT
U2IN = U2OUT
W2IN = W2OUT
U1K2 = U1(K2)
U2K2 = U2(K2)
W1K2 = W1(K2)
W2K2 = W2(K2)
DU1IN = DU1OUT
DU2IN = DU2OUT
DW1IN = DW1OUT
DW2IN = DW2OUT

C

START OUTWARD INTEGRATION

C

U1 = 1*D - 10
U2 = 1*D - 10
W1 = U1*RS1
W2 = U2*RS2

C

K = 0
K1 = 1
L1 = JOUT
L2 = 1
GO TO 135

C

197 U1(K1) = U1K2
U2(K1) = U2K2
W1(K1) = W1K2
W2(K1) = W2K2

198 GO TO (199 + Z31) * ICC

C

OUTWARD U SOLUTION = B(1) * U1 + B(2) * U2
OUTWARD W SOLUTION = B(1) * W1 + B(2) * W2
INWARD U SOLUTION = B(3) * U1 + U2
INWARD W SOLUTION = B(3) * W1 + W2
MATCHING POINT CONDITIONS ARE

C

C

B11 * U1OUT + B(2) * U2OUT = B(3) * U1IN + U2IN
B11 * W1OUT + B(2) * W2OUT = B(3) * W1IN + W2IN
B11 * DU1OUT + B(2) * DU2OUT = B(3) * DU1IN + DU2IN
B11 * DW1OUT + B(2) * DW2OUT = B(3) * DW1IN + DW2IN

C

199 C = 1*D0 / U2IN
B = 1*D0
B(2) = W2IN*C

C

A(1 + 1) = U1OUT*C
A(1 + 2) = U2OUT*C
A(1 + 3) = -U1IN*C
A(2*1)=W1OUT*C
A(2*2)=W2OUT*C
A(2*3)=W1IN*C
C
201 GO TO (205,209),M
205 B(3)=DU2IN*C
A(3*1)=DU1OUT*C
A(3*2)=DU2OUT*C
A(3*3)=DU1IN*C
GO TO 213
C
209 B(3)=DW2IN*C
A(3*1)=DW1OUT*C
A(3*2)=DW2OUT*C
A(3*3)=DW1IN*C
C
213 CALL SYSTEM(A+3,B)
C
221 GO TO (225,229),M
225 WM=B(3)*W1IN+W2IN
GO TO 237
229 UM=B(3)*U1IN+U2IN
237 GO TO (241,257,242,257,257),IPR
C
C OUTWARD U SOLUTION (E=0°) = B(1)*U1+B(2)*U2
C OUTWARD W SOLUTION (E=0°) = B(1)*W1+B(2)*W2
C INWARD U SOLUTION (E=0°) = B(3)*U1+B(4)*U2+U3
C INWARD W SOLUTION (E=0°) = B(3)*W1+B(4)*W2+W3
C
C MATCHING POINT CONDITIONS (E=0°) ARE
C B(1)*U1OUT+B(2)*U2OUT=B(3)*U1IN+B(4)*U2IN+U3IN
C B(1)*W1OUT+B(2)*W2OUT=B(3)*W1IN+B(4)*W2IN+W3IN
C B(1)*DU1OUT+B(2)*DU2OUT=B(3)*DU1IN+B(4)*DU2IN+DU3IN
C B(1)*DW1OUT+B(2)*DW2OUT=B(3)*DW1IN+B(4)*DW2IN+DW3IN
231 C=I.DO/1l311
A=I.DO
B(2)=W3IN*C
B(3)=DU3IN*C
B(4)=DW3IN*C
C
A(1*1)=U1OUT*C
A(1*2)=U2OUT*C
A(1*3)=U1IN*C
A(1*4)=U2IN*C
C
A(2*1)=W1OUT*C
A(2*2)=W2OUT*C
A(2*3)=W1IN*C
A(2*4)=W2IN*C
C
A(3*1)=DU1OUT*C
A(3*2)=DU2OUT*C
A(3*3)=DU1IN*C
A(3*4)=DU2IN*C
A(4,1) = DW1OUT*C
A(4,2) = DW2OUT*C
A(4,3) = -DW1IN*C
A(4,4) = -DW2IN*C

C
CALL SYSTEM(A, 4*B)
C
B1 = 1.00/(B(3) + B(4) + 1.00)
B = B1*B
B(2) = B1*B(2)
B(3) = B1*B(3)
B(4) = B1*B(4)

C
GO TO (244, 257, 244, 257), IPR
C
IF (IT - MAXIT) 257, 242, 242
C
IF (IT = 1) 244, 244, 243
WRITE (6, 522)
I1 = 0
C
DO 1247 JF = 1, NT, 300
   IF (II) 245, 245, 1244
1244 WRITE (6, 522)
DO 245 WRITE (6, 524)
   JL = MIN0(JF + 49, NT)
   DO 246 J1 = JF, JL
   IL = MIN0(J1 + 250, NT)
246 WRITE (6, 540)(R(L), U1(L), L = J1, IL, 50)
1246 II = II + 1
C
DO 247 JF = 1, NT, 300
WRITE (6, 528)
   JL = MIN0(JF + 49, NT)
   DO 247 J1 = JF, JL
   IL = MIN0(J1 + 250, NT)
247 WRITE (6, 540)(R(L), U2(L), L = J1, IL, 50)
C
GO TO (250, 248), ICC
248 DO 249 JF = NT4, NT, 300
WRITE (6, 530)
   JL = MIN0(JF + 49, NT)
   DO 249 J1 = JF, JL
   IL = MIN0(J1 + 250, NT)
249 WRITE (6, 540)(R(L), U3(L), L = J1, IL, 50)
C
DO 251 JF = 1, NT, 300
WRITE (6, 532)
   JL = MIN0(JF + 49, NT)
   DO 251 J1 = JF, JL
   IL = MIN0(J1 + 250, NT)
251 WRITE (6, 540)(R(L), W1(L), L = J1, IL, 50)
C
DO 252 JF = 1, NT, 300
WRITE (6, 536)
JL=MINO(JF+49,NT)
DO 252 J1=JF, JL
IL=MINO(J1+250,NT)
WRITE (6,540)(R(L), W2(L), L=J1,IL,50)
C
GO TO (257,253),ICC
DO 254 JF=NT4,NT,300
WRITE (6,538)
JL=MINO(JF+49,NT)
DO 254 J1=JF, JL
IL=MINO(J1+250,NT)
WRITE (6,540)(R(L), W3(L), L=J1,IL,50)
C
SOLUTIONS
C
GO TO (257,329),ICC
DO 265 L=1,NT3
U(L)=B*U1(L)+B(2)*U2(L)
W(L)=B*W1(L)+B(2)*W2(L)
U2S(L)=SIMP(L)*U(L)*U(L)
W2S(L)=SIMP(L)*W(L)*W(L)
C1=C1+U2S(L)
C2=C2+W2S(L)
C
GO TO (269,329),ICC
DO 273 L=NT2,NT1
U(L)=B(3)*U1(L)+U2(L)
W(L)=B(3)*W1(L)+W2(L)
U2S(L)=SIMP(L)*U(L)*U(L)
W2S(L)=SIMP(L)*W(L)*W(L)
C1=C1+U2S(L)
C2=C2+W2S(L)
U(NT)=B(3)*U1(NT)+U2(NT)
W(NT)=B(3)*W1(NT)+W2(NT)
U2S(NT)=(SIMP(NT)+P1)*U(NT)*U(NT)
W2S(NT)=(SIMP(NT)+P2)*W(NT)*W(NT)
C1=C1+U2S(NT)
C2=C2+W2S(NT)
C3=C1+C2
C
ENERGY CORRECTOR FORMULA
C
GO TO (289,293),M
F=(B*DW1OUT+B(2)*DW2OUT-B(3)*DW1IN-DW2IN)*WM
GO TO 297
F=(B*DU1OUT+B(2)*DU2OUT-B(3)*DU1IN-DU2IN)*UM
DE=F*A1
C
WRITE (6,544)IT, E0, EE, DE, B(1), B(2), B(3)
C
EE=EE+DE
IF(EE) GO TO 305
WRITE (6,564)
DE=DE-EE
GO TO 409
309 ED=EE/HTM
K1=IT-MAXIT
C
313 IF(DABS(DE)-DABS(EPS)*HTM).GT.317,321,321
317 K1=0
C
NORMALIZE
C
321 A2=DSORT(A1)
323 DO 325 L=1,NT
U(L)=U(L)*A2
325 W(L)=W(L)*A2
337 GO TO (341,341,345,345,353)*IPR
C
329 DO 331 L=NT2,NT1
U(L)=B(3)*U1(L)+B(4)*U2(L)+B1*U3(L)
W(L)=B(3)*W1(L)+B(4)*W2(L)+B1*W3(L)
U2S(L)=SIMP(L)*U(L)*U(L)
331 W2S(L)=SIMP(L)*W(L)*W(L)
U1NT)=B(3)*U1(NT)+B(4)*U2(NT)+B1*U3(NT)
W(NT)=B(3)*W1(NT)+B(4)*W2(NT)+B1*W3(NT)
U2SNT)=SIMP(NT)*U(NT)*U(NT)
W2SNT)=SIMP(NT)*W(NT)*W(NT)
GO TO (345,345,345,353)*IPR
C
341 IF(K1).LT.353,345,345
345 DO 347 JF=1,NT,300
WRITE (6,548)
JL=MINO(JF+49,NT)
DO 347 JF=JF+JL
1L=MINO(JF+250,NT)
347 WRITE (6,540)(R(L),U(L),L=J1,IL,50)
C
DO 349 JF=1,NT,300
WRITE (6,552)
JL=MINO(JF+49,NT)
DO 349 JF=JF+JL
IL=MINO(JF+250,NT)
349 WRITE (6,540)(R(L),W(L),L=J1,IL,50)
C
353 GO TO (357,397),1CC
357 IF(K1).GE.361,377,377
361 RF2=(B(3)*RF1+RF2)/(B(3)+1,DO)
373 RS2=(B*RS1+B(2)*RS2)/(B+B(2))
C
PERCENTAGE D-STATE AND QUADRUPOLE MOMENT
C
377 PD=C2*A1
B2=RAD2+RAD2
Q=0.0
381 DO 385 L=1,NT1
385 Q=Q+SIMP(L)*W(L)*R(L)*R(L)*(B2*U(L)-W(L))
Q=Q+0.05DO*(Q+(SIMP(NT)+P3)*B2*U(NT)-(SIMP(NT)+P4)*W(NT))*W(NT)
WRITE (6,556) E0,O,PD
WRITE (6,522)  
DE=DE-EE
GO TO (409,393),IC

393  
ICC=2
A=P*RI)
B=1+DO/A
R=1+DO/P-2*DO*DEXP(-A)/RI)+RI)+(RI)/RI+3*DO*B*(1+DO)
GO TO 89  

C  
SCATTERING LENGTH AND EFFECTIVE RANGE  
397  
SCL=1+DO/(GI*(B1+B(3)))+G2*B(4))
A=R/RI)/SCL
ROT=R/RI)*RI+DO-A*(RI+DO-A/3+DO)
403 DO 405 L=1+NT
405 ROT=ROT-U2S(L)-W2S(L)
ROT=ROT+ROT  
C  
IF(ICC=2) GO TO 406,407,406
406 WRITE (6,560) SCL, ROT
WRITE (6,522)  
GO TO 408  
C  
407 A=DSQRT(EE)-1+DO/SCL
B=1+DO/(EE*EE*ROT**3)
ASDP=(A+B+5DO*EE*ROT)*B
SDP=(3+DO*A+EE*(ROT+0.5DO*ROT))%B
AMFR=(A-A)/EE
SSP=(-AMFR+0.5DO*(ROT+ROT))/B/(ROT*ROT)
WRITE (6,562) SCL, ROT, SDP, AMFR, R, ASDP, SSP
C  
408 DE=0+DO
GO TO (12,4,61),IR  
C  
END  
SIBFTC PODD NOLIST DECK  
DIMENSION N(10),H(10),HV(10),X(10),R(300),F1(300),F2(300),F3(300)
COMMON H,HTM,RAD2  
C  
DOUBLE PRECISION H,X,R,F1  
DOUBLE PRECISION F2,F3,CC1,VC,HTM  
DOUBLE PRECISION CT1,VT,CL1,VL,A  
DOUBLE PRECISION DEXP,RC,RT,RL,H1  
DOUBLE PRECISION B,B6,ECH,ETH,ELM  
DOUBLE PRECISION EC1,ET1,EL1,CC,CT  
DOUBLE PRECISION CL,RAD2,DFLOAT  
DFLOAT(11)=1  
C  
IV=1+2+3+4 FOR SQUARE, EXPONENTIAL, YUKAWA AND GAUSS WELL  
POTENTIALS RESPECTIVELY  
C  
GO TO (1+5+5+9),IV  
1 CC1=VC*HTM  
CT1=(VT+VT)*HTM  
CL1=3+DO*VL*HTM  
C
M1=1
M2=1
M3=1
GO TO 13

C 5
A=R-H
CC1=VC*DEXP(-RC*A)*HTM
CT1=(VT+VT)*DEXP(-RT*A)*HTM
CL1=3.00*VL*DEXP(-RL*A)*HTM

C 11
IF(IV-3)13,11,11
CC1=CC1/RC
CT1=CT1/RT
CL1=CL1/RL
GO TO 13

C 9
A=R-H
CC1=VC*DEXP(-RC*A*A)*HTM
CT1=(VT+VT)*DEXP(-RT*A*A)*HTM
CL1=3.00*VL*DEXP(-RL*A*A)*HTM

C 13
K=0
DO 109 L=1,JTOT
NL=N(L)
H1=H(L)
B=HV(L)
B6=6.00*D6

C 21
GO TO (33,25,25,29)*IV
25 ECH=DEXP(-RC*H1)
ETH=DEXP(-RT*H1)
ELH=DEXP(-RL*H1)
GO TO 33

C 29
ECH=DEXP(-RC*(A+H1))
ETH=DEXP(-RT*(A+H1))
ELH=DEXP(-RL*(A+H1))
EC1=DEXP(-RC*H1*H1)
ET1=DEXP(-RT*H1*H1)
EL1=DEXP(-RL*H1*H1)

C 33
DO 97 IB=1,NL
K=K+1

C 37
GO TO (41,77,69,81)*IV
41 GO TO (45,53,57,49,49)
45 IF(R(KI)-RCI53,49,49
49 M1=2
CC1=0.00*D0

C 53
GO TO (57,65,61,61)
57 IF(R(KI)-RTI65,61,61
61 M2=2
CT1=0.00*D0

C 65
GO TO (69,85,73,73)
69 IF(R(KI)-RLI85,73,73
73 M3=2
CL1=0.00*D0
GO TO 85

C 77
CC1=CC1*ECH
CT1=CT1*ETH
CL1=CL1*ELH
GO TO 85

C
81  CC1=CC1*ECH*EC1
    CT1=CT1*ETH*ET1
    CL1=CL1*ELH*EL1
    ECH=ECH*EC1*EC1
    ETH=ETH*ET1*ET1
    ELH=ELH*EL1*EL1

85  CC=CC1*A
    CT=CT1*B
    CL=CL1*B
    GO TO 93

89  CC1=CC1*ECH
    CT1=CT1*ETH
    CL1=CL1*ELH
    A=B/R(K)
    CC=CC1*A
    CT=CT1*A
    CL=CL1*A

93  F1(K)=CC
    F2(K)=CT*RAD2

97  F3(K)=CC-CT-CL + B6/(R(K)*R(K))

101  GO TO (109,109,109,105),IV

15  A=A+H1*DFLOAT(NL)

109  CONTINUE

C

113  NL=NL+M(L)
    M1=JOUT+1
    M2=JOUT-1
    DO 117 L=M1,M2
    NL=NL+M(L)
    B=X(L)*X(L)
    F1(NL)=B*F1(NL)
    F2(NL)=B*F2(NL)

117  F3(NL)=B*F3(NL)
    RETURN

END
APPENDIX B

LISTING OF A SAMPLE SET OF DATA

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<th>0.001+0</th>
<th>4</th>
<th>6</th>
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<td>5.0+0</td>
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<td>2.5+0</td>
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<td>2.0</td>
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<tr>
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<td>3.0</td>
<td>5.0</td>
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<td>2.0+0</td>
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### SOLUTION OF SCHROEDINGER DEUTERON EQUATION

#### INITIAL PARAMETER VALUES

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<th>NUMBER OF BLOCKS</th>
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<tbody>
<tr>
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<td>0.100000d-02</td>
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#### INWARD INTEGRATION - NUMBER OF BLOCKS JOUT = 4

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<th>H</th>
<th>X</th>
<th>N</th>
<th>H</th>
<th>X</th>
<th>N</th>
<th>H</th>
<th>X</th>
<th>N</th>
<th>H</th>
<th>X</th>
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<td>0.40000d-02</td>
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<td>0.50000d-01</td>
<td>0.10000d-01</td>
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#### MATCHING POINT ABSCISSA = 0.17800d-01

#### INWARD INTEGRATION - NUMBER OF BLOCKS JIN = 2

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#### PARAMETERS SPECIFYING POTENTIAL

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<tr>
<th>IV</th>
<th>VC</th>
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<th>VT</th>
<th>RT</th>
<th>VL</th>
<th>RL</th>
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#### REMAINING DATA SPECIFYING SOLUTION

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<th>IC</th>
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<th>G1</th>
<th>G2</th>
<th>G3</th>
<th>RF1</th>
<th>RF2</th>
<th>RS1</th>
<th>KL2</th>
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<td>2</td>
<td>-0.100000d-01</td>
<td>-0.300000d-00</td>
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IT= 1 Ed= -2.0000000D 00 OC EE= -4.62286000D-03 DE= -4.80827170D-03 N(1/3)= 9.76543690D-01 -4.79546360D-01 2.94124340D-01

IT= 2 Ed= -2.1993950D 00 OC EE= -5.30368720D-02 DE= -9.67923590D-05 B(1/3)= 1.13686390-10 7.83197+20-02 1.96591730 00

IT= 3 Ed= -2.2034890D 00 OC EE= -5.31336640D-02 DE= -3.50679360D-04 B(1/3)= 8.32692860-13 2.75331730-02 3.9736120-02

IT= 4 Ed= -2.20341040D 00 OC EE= -5.31336990D-02 DE= 6.3274280-15 B(1/3)= 2.83539750D-16 2.64821570-02 1.4375420-05

IT= 5 Ed= -2.20341040D 00 OC EE= -5.31336990D-02 DE= -1.34217160-14 B(1/3)= 3.92876520-18 2.64817770-02 1.91979580-12

IT= 6 Ed= -2.20341640D 00 OC EE= -5.31336990D-02 DE= 2.63193230-14 B(1/3)= 1.56383080D-19 2.64817770-02 -3.10326150D-12

IT= 7 Ed= -2.20341040D 00 OC EE= -5.31336990D-02 DE= -1.64605290D-15 B(1/3)= 5.08909730D-19 2.64817770-02 -4.67504320D-12
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### SCATTERING LENGTH

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<th>EFFECTIVE RANGE</th>
<th>SHAPE PARAMETER</th>
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<td>0.374300 CC</td>
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### MIXED EFFECTIVE RANGE

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<th>DEUTERON EFFECTIVE RANGE</th>
<th>APPROX. SHAPE PARAMETER</th>
<th>SECOND SHAPE PARAMETER</th>
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<tbody>
<tr>
<td>0.319400 CC</td>
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