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UNITED STATES
ATOMIC ENERGY COMMISSION
CONTRACT W-7405-ENG. 36

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Printed in the United States of America. Available from
Clearinghouse for Federal Scientific and Technical Information
National Bureau of Standards, U. S. Department of Commerce
Springfield, Virginia 22151
Price: Printed Copy $3.00; Microfiche $0.65

LA-3949
UC-34, PHYSICS
TID-4500

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Report written: May 1968
Report distributed: October 1, 1968

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by

Gerald G. Ohlsen

MAJORANA DEPOLARIZATION OF HYDROGEN, DEUTERIUM, OR TRITIUM ATOMS

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ABSTRACT

The theory required to follow the behavior of a hydrogen, deuterium, or tritium atom in a time-dependent magnetic field is described. A computer code is included, and some numerical results of interest to the design of Lamb-shift polarized-ion sources are presented. A brief discussion of depolarization effects in pick-up or stripping of two electrons is also presented.

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1. INTRODUCTION

In all sources of polarized hydrogen or deuterium ions which have been proposed, the process involves, first, the production of a beam of atoms with a net nuclear polarization and, second, the ionization of these polarized atoms. It is frequently required to change the magnetic field strength or direction or both from one value to another between the point at which the polarized atoms are produced and that at which they are ionized. Thus, one is required, in the design of such devices, to estimate depolarization effects caused by unwanted transitions between the various hyperfine states when atoms are subjected to time-varying magnetic fields. (Such transitions are usually referred to as Majorana transitions.) In most cases one wishes to design magnetic field shapes in a way which eliminates or reduces these effects. Problems of this type are particularly important in "Lamb-shift" sources, where the atomic beam velocities are large ($\sim$30 cm/μsec).

A related problem, which we will also consider, is the "zero field crossing" technique of polarization enhancement. In this method it is required to reverse the direction of the magnetic field in a way such that a certain transition is made with high probability while the remaining transitions occur with low probability. We will also briefly discuss the depolarization of ions that may occur when two electrons are stripped or picked up, as in a tandem accelerator stripper or a cesium adding canal.

2. THEORY

The Schroedinger equation for a one-electron atom may be written

$$(H_o + H_1)\Psi = i\hbar \frac{\partial \Psi}{\partial t} , \qquad (1)$$

where H_o is that part of the Hamiltonian which does not depend on electronic or on nuclear spin and where

$$H_1 = (\mu_o g_J \vec{J} + \mu_N g_I \vec{I}) \cdot \vec{B} + \alpha(\vec{I}\cdot\vec{J}) . \qquad (2)$$

In the above expression $\mu_o = e\hbar/2mc$ (the Bohr magneton); $\mu_N = e\hbar/2m_p c$ (the nuclear magneton); g_J and g_I are the electronic and nuclear g-factors, respectively; and α is related as follows to the zero field hyperfine energy separation (ΔW):

$$\begin{aligned} \alpha &= \Delta W/I(2J + 1) \text{ if } I < J \\ &= \Delta W/J(2I + 1) \text{ if } J < I . \end{aligned} \qquad (3)$$

For hydrogen atoms $I = J = 1/2$ and thus $\alpha = \Delta W$; for deuterium atoms $I = 1$, $J = 1/2$, and therefore $\alpha = 2\,\Delta W/3$.

If we assume a complete set of functions u_n which satisfy $H_o u_n = E_o u_n$, we may write the general wave function as

$$\Psi = \Sigma b_n u_n e^{-iE_o t/\hbar} . \qquad (4)$$

We consider the u_n to be the four strong field states $\Psi(m_I, m_J)$ for hydrogen atoms (six states for deuterium atoms), where the quantization axis is specified and stationary and where m_I and m_J are the nuclear and electronic magnetic quantum numbers, respectively. All of these states have the same space wave function and, hence, the same eigenvalue of the operator H_o. Substituting Eq. 4 into Eq. 1, multiplying from the left by u_m^*, and integrating over the space variables, we obtain the equations of motion of the probability amplitudes:

$$i\hbar \dot{b}_m = \Sigma b_n \langle u_m | H_1 | u_n \rangle . \qquad (5)$$

If we put explicit values of the matrix elements into the above expression and use the quantum numbers m_I and m_J to label the states, Eq. 5 becomes[1]

$$i\hbar \dot{b}_{m_I,m_J} = [(\mu_o g_J m_J + \mu_N g_I m_I)B_z + \alpha m_I m_J] b_{m_I,m_J} \qquad (6)$$

$$+\tfrac{1}{2}\mu_o g_J (B_x - iB_y)[(J-m_J)(J+m_J+1)]^{\frac{1}{2}} b_{m_I,m_J+1}$$

$$+\tfrac{1}{2}\mu_o g_J (B_x + iB_y)[(J+m_J)(J-m_J+1)]^{\frac{1}{2}} b_{m_I,m_J-1}$$

$$+\tfrac{1}{2}\mu_N g_I (B_x - iB_y)[(I-m_I)(I+m_I+1)]^{\frac{1}{2}} b_{m_I+1,m_J}$$

$$+\tfrac{1}{2}\mu_N g_I (B_x + iB_y)[(I+m_I)(I-m_I=1)]^{\frac{1}{2}} b_{m_I-1,m_J}$$

$$+\tfrac{1}{2}\alpha[(I-m_I)(I+m_I+1)(J+m_J)(J-m_J+1)]^{\frac{1}{2}} b_{m_I+1,m_J-1}$$

$$+\tfrac{1}{2}\alpha[(I+m_I)(I-m_I+1)(J-m_J)(J+m_J+1)]^{\frac{1}{2}} b_{m_I-1,m_J+1} ,$$

where g_I is the nuclear and g_J is the electronic g-factor (see Table I). We define the following parameters:

$$k = \frac{g_I}{1836.1\, g_J} \qquad (7)$$

$$B_o = \frac{\alpha}{\mu_o g_J} .$$

With these definitions Eq. 6 reduces, for hydrogen or tritium atoms, to the following four coupled differential equations:

$$\begin{bmatrix} \dot{b}_1 \\ \dot{b}_2 \\ \dot{b}_3 \\ \dot{b}_4 \end{bmatrix} = \frac{\mu_o g_J}{i\hbar} \begin{bmatrix} \tfrac{1}{2}(1+k)B_z + \tfrac{1}{4}B_o & \tfrac{1}{2}kB_+ & 0 & \tfrac{1}{2}B_+ \\ \tfrac{1}{2}kB_- & \tfrac{1}{2}(1-k)B_z - \tfrac{1}{4}B_o & \tfrac{1}{2}B_+ & \tfrac{1}{2}B_o \\ 0 & \tfrac{1}{2}B_- & -\tfrac{1}{2}(1+k)B_z + \tfrac{1}{4}B_o & \tfrac{1}{2}kB_- \\ \tfrac{1}{2}B_- & \tfrac{1}{2}B_o & \tfrac{1}{2}kB_+ & -\tfrac{1}{2}(1-k)B_z - \tfrac{1}{4}B_o \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix} , \qquad (8)$$

TABLE I

HYPERFINE STRUCTURE PARAMETERS

State	g_I	g_J	ε	B_1	ΔW	k	B_o
1S Hydrogen	5.585486	2.00229	1.522×10^{-3}	507.591	1420.406	1.520×10^{-3}	506.820
2S Hydrogen	5.585486	2.00229	1.522×10^{-3}	63.450	177.557	1.520×10^{-3}	63.354
1S Deuterium	0.857407	2.00229	0.233×10^{-3}	116.842	327.384	0.233×10^{-3}	77.877
2S Deuterium	0.857407	2.00229	0.233×10^{-3}	14.605	40.924	0.233×10^{-3}	9.735
1S Tritium	5.957680	2.00229	1.623×10^{-3}	542.059	1516.702	1.620×10^{-3}	541.181
2S Tritium	5.957680	2.00229	1.623×10^{-3}	67.759	189.594	1.620×10^{-3}	67.650

where B_x, B_y, and B_z are the components of the applied B field (arbitrary time variation), $B_+ = B_x + iB_y$, $B_- = B_x - iB_y$, and states 1-4 are the strong field states $\Psi(m_I, m_J)$ ordered according to their energy in a magnetic field (as indicated in Fig. 1). For deuterium atoms Eq. 6 reduces to six coupled differential equations:

$$\begin{bmatrix} \dot{b}_1 \\ \dot{b}_2 \\ \dot{b}_3 \\ \dot{b}_4 \\ \dot{b}_5 \\ \dot{b}_6 \end{bmatrix} = \frac{\mu_o g_J}{i\hbar} \begin{bmatrix} (\tfrac{1}{2}+k)B_z+\tfrac{1}{2}B_o & kB_+ & 0 & 0 & 0 & \tfrac{1}{2}B_+ \\ kB_- & \tfrac{1}{2}B_z & kB_+ & 0 & \tfrac{1}{2}B_+ & B_o/\sqrt{2} \\ 0 & kB_- & (\tfrac{1}{2}-k)B_z-\tfrac{1}{2}B_o & \tfrac{1}{2}B_+ & B_o/\sqrt{2} & 0 \\ 0 & 0 & \tfrac{1}{2}B_- & -(\tfrac{1}{2}+k)B_z+\tfrac{1}{2}B_o & kB_- & 0 \\ 0 & \tfrac{1}{2}B_- & B_o/\sqrt{2} & kB_+ & -\tfrac{1}{2}B_z & kB_- \\ \tfrac{1}{2}B_- & B_o/\sqrt{2} & 0 & 0 & kB_+ & -(\tfrac{1}{2}-k)B_z-\tfrac{1}{2}B_o \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \\ b_6 \end{bmatrix} , \quad (9)$$

where the states 1-6 are the strong field states ordered as described above (as indicated in Fig. 2). The parameter k is a small number ($\sim 10^{-3}$) and thus could be neglected for most purposes, although this assumption has not been made in the numerical calculations to be described in subsequent sections.

We note in passing that the parameters k and B_o are different from those which arise in the description of the energy levels of the atom. Specifically, the "Breit-Rabi formula" for hydrogen or tritium atoms is

$$W = -\tfrac{1}{4}\Delta W \pm \tfrac{1}{2}\Delta W(1+2m_F x+x^2)^{\frac{1}{2}} + \varepsilon \Delta W m_F x \ , \quad (10)$$

where $m_F = m_I + m_J$ and where the plus sign applies to states 1, 2, and 3 while the minus sign applies to state 4. The quantity $x = B/B_1$, with $B_1 = \Delta W/[(1-k)\mu_o g_J] \equiv B_o/(1-k)$ and $\varepsilon = k/(1-k)$. For deuterium atoms we have

$$W = -\frac{1}{6}\Delta W \pm \frac{1}{2}\Delta W(1+\frac{4}{3}m_F x+x^2)^{\frac{1}{2}} + \varepsilon \Delta W m_F x \ . \quad (11)$$

The definitions of x and of ε remain the same, but in this case we have $B_1 = 3B_o/[2(1-k)]$. The plus sign applies to states 1-4 while the minus sign applies to states 5-6. The numerical values of the parameters used in Eqs. 8-11 are given in Table I.

The solution of the above differential equa-

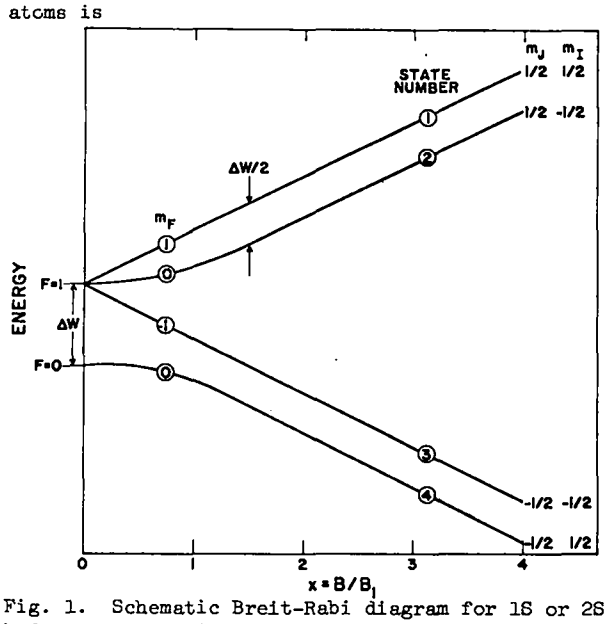

Fig. 1. Schematic Breit-Rabi diagram for 1S or 2S hydrogen or tritium atoms.

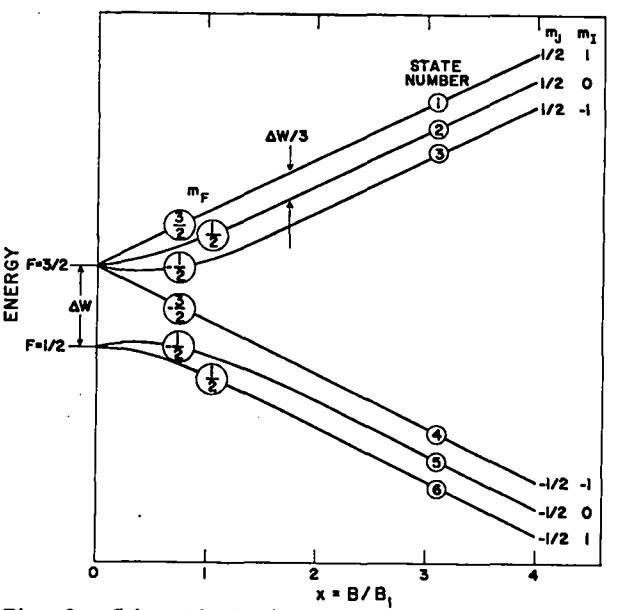

Fig. 2. Schematic Breit-Rabi diagram for 1S or 2S deuterium atoms.

tions (Eqs. 8 or 9) for the field variation of interest, then, is a straightforward computational problem. However, the states we have used in the description are the strong field states with respect to a fixed z-axis. Since, in general, the direction of the magnetic field varies, it is somewhat easier to interpret the results if the coordinate system is rotated, so that the new z-axis lies along the (time-varying) magnetic field direction. The rotation transformation for composite states may be derived from the spin-1/2 and spin-1 rotation matrices. For a spin-1/2 particle, the rotation transformation may be represented by the matrix equation

$$\begin{bmatrix} b'_+ \\ b'_- \end{bmatrix} = \begin{bmatrix} a_{++} & a_{+-} \\ a_{-+} & a_{--} \end{bmatrix} \begin{bmatrix} b_+ \\ b_- \end{bmatrix} , \qquad (12)$$

where the subscript refers to the sign of the magnetic quantum number $m(=\pm\frac{1}{2})$. Explicitly, the coefficients are

$$\begin{aligned} a_{++} &= \cos(\tfrac{1}{2}\beta)\exp[-\tfrac{1}{2}i(\alpha+\gamma)] \\ a_{--} &= \cos(\tfrac{1}{2}\beta)\exp[\tfrac{1}{2}i(\alpha+\gamma)] \\ a_{-+} &= -\sin(\tfrac{1}{2}\beta)\exp[-\tfrac{1}{2}i(\alpha-\gamma)] \\ a_{+-} &= \sin(\tfrac{1}{2}\beta)\exp[\tfrac{1}{2}i(\alpha-\gamma)] , \end{aligned} \qquad (13)$$

$$\begin{bmatrix} b'_1 \\ b'_2 \\ b'_3 \\ b'_4 \\ b'_5 \\ b'_6 \end{bmatrix} = \begin{bmatrix} a_{++}c_{++} & a_{++}c_{+o} & a_{++}c_{+-} \\ a_{++}c_{o+} & a_{++}c_{oo} & a_{++}c_{o-} \\ a_{++}c_{-+} & a_{++}c_{-o} & a_{++}c_{--} \\ a_{-+}c_{-+} & a_{-+}c_{-o} & a_{-+}c_{--} \\ a_{-+}c_{o+} & a_{-+}c_{oo} & a_{-+}c_{o-} \\ a_{-+}c_{++} & a_{-+}c_{+o} & a_{-+}c_{+-} \end{bmatrix}$$

where α, β, and γ are the positive Euler angles[2] which rotate the initial coordinate system (unprimed) into the final coordinate system (primed). For hydrogen or tritium atoms (in strong field representation), the rotation matrix is essentially a direct product of the electronic and nuclear rotation. The complete rotation matrix may be written

$$\begin{bmatrix} b'_1 \\ b'_2 \\ b'_3 \\ b'_4 \end{bmatrix} = \begin{bmatrix} a_{++}a_{++} & a_{++}a_{+-} & a_{+-}a_{+-} & a_{+-}a_{++} \\ a_{++}a_{-+} & a_{++}a_{--} & a_{+-}a_{--} & a_{+-}a_{-+} \\ a_{-+}a_{-+} & a_{-+}a_{--} & a_{--}a_{--} & a_{--}a_{-+} \\ a_{-+}a_{++} & a_{-+}a_{+-} & a_{--}a_{+-} & a_{--}a_{++} \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix} , \qquad (14)$$

where states 1-4 are ordered as in Fig. 1. (Note that the states 3 and 4 are interchanged in relation to the notation one would choose if a true direct product notation were to be applicable.) For a spin-1 particle, the rotation matrix is

$$\begin{bmatrix} b'_+ \\ b'_o \\ b'_- \end{bmatrix} = \begin{bmatrix} c_{++} & c_{+o} & c_{+-} \\ c_{o+} & c_{oo} & c_{o-} \\ c_{-+} & c_{-o} & c_{--} \end{bmatrix} \begin{bmatrix} b_+ \\ b_o \\ b_- \end{bmatrix} \qquad (15)$$

in an obvious notation. In this case the coefficients are given by

$$\begin{aligned} c_{++} &= (\tfrac{1}{2}+\tfrac{1}{2}\cos\beta)\exp[-i(\alpha+\gamma)] \\ c_{+o} &= (\sin\beta/\sqrt{2})\exp[-i\gamma] \\ c_{+-} &= (\tfrac{1}{2}-\tfrac{1}{2}\cos\beta)\exp[i(\alpha-\gamma)] \\ c_{o+} &= -(\sin\beta/\sqrt{2})\exp[-i\alpha] \\ c_{oo} &= \cos\beta \\ c_{o-} &= (\sin\beta/\sqrt{2})\exp[i\alpha] \\ c_{-+} &= (\tfrac{1}{2}-\tfrac{1}{2}\cos\beta)\exp[-i(\alpha-\gamma)] \\ c_{-o} &= -(\sin\beta/\sqrt{2})\exp[i\gamma] \\ c_{--} &= (\tfrac{1}{2}+\tfrac{1}{2}\cos\beta)\exp[i(\alpha+\gamma)]. \end{aligned} \qquad (16)$$

The complete rotation matrix for a deuterium atom may be written

$$\begin{bmatrix} b'_1 \\ b'_2 \\ b'_3 \\ b'_4 \\ b'_5 \\ b'_6 \end{bmatrix} = \begin{bmatrix} a_{+-}c_{+-} & a_{+-}c_{+o} & a_{+-}c_{++} \\ a_{+-}c_{o-} & a_{+-}c_{oo} & a_{+-}c_{o+} \\ a_{+-}c_{--} & a_{+-}c_{-o} & a_{+-}c_{-+} \\ a_{--}c_{--} & a_{--}c_{-o} & a_{--}c_{-+} \\ a_{--}c_{o-} & a_{--}c_{oo} & a_{--}c_{o+} \\ a_{--}c_{+-} & a_{--}c_{+o} & a_{--}c_{++} \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \\ b_6 \end{bmatrix} , \qquad (17)$$

where the states 1-6 are ordered as in Fig. 2.

Finally, it is usually more convenient to describe the final system in terms of eigenstates of the particular magnetic field strength rather than in terms of the strong field eigenstates. If the fields are changed slowly enough, the system will remain in a particular state; that is, the energy of the system will remain on one of the lines 1-4 for hydrogen atoms or 1-6 for deuterium atoms (provided that, initially, the system was in such an eigenstate). These eigenstates are, in general, linear combinations of the strong field basis states used in Eqs. 8 and 9. In terms of these "intermediate

field" states, failures of adiabaticity will appear in the form of transitions from the initial state (or the state to which it would have been transformed if the process were adiabatic) to one or more of the other states. In terms of the strong field state amplitudes (primed), the amplitudes of the hydrogen or tritium atom intermediate-field eigenstates (double-primed) may be written, for arbitrary B, as

$$\begin{bmatrix} b''_1 \\ b''_2 \\ b''_3 \\ b''_4 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \sqrt{\tfrac{1}{2}(1+\delta)} & 0 & \sqrt{\tfrac{1}{2}(1-\delta)} \\ 0 & 0 & 1 & 0 \\ 0 & -\sqrt{\tfrac{1}{2}(1-\delta)} & 0 & \sqrt{\tfrac{1}{2}(1+\delta)} \end{bmatrix} \begin{bmatrix} b'_1 \\ b'_2 \\ b'_3 \\ b'_4 \end{bmatrix}, \quad (18)$$

where $\delta = x/(1+x^2)^{\frac{1}{2}}$ and $x = B/B_1$. For deuterium atoms we have

$$\begin{bmatrix} b''_1 \\ b''_2 \\ b''_3 \\ b''_4 \\ b''_5 \\ b''_6 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \sqrt{\tfrac{1}{2}(1+\delta_+)} & 0 & 0 & 0 & \sqrt{\tfrac{1}{2}(1-\delta_+)} \\ 0 & 0 & \sqrt{\tfrac{1}{2}(1+\delta_-)} & 0 & \sqrt{\tfrac{1}{2}(1-\delta_-)} & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -\sqrt{\tfrac{1}{2}(1-\delta_-)} & 0 & \sqrt{\tfrac{1}{2}(1+\delta_-)} & 0 \\ 0 & -\sqrt{\tfrac{1}{2}(1-\delta_+)} & 0 & 0 & 0 & \sqrt{\tfrac{1}{2}(1+\delta_+)} \end{bmatrix} \begin{bmatrix} b'_1 \\ b'_2 \\ b'_3 \\ b'_4 \\ b'_5 \\ b'_6 \end{bmatrix}, \quad (19)$$

where

$$\delta_+ = (x+1/3)/(1+2x/3+x^2)^{\frac{1}{2}}$$
$$\delta_- = (x-1/3)/(1-2x/3+x^2)^{\frac{1}{2}}$$

and again $x = B/B_1$. From these eigenfunctions one can easily calculate the nuclear and electronic polarization of a beam whose atoms are in a particular pure state (see Table II).

The nuclear polarization parameters may be written in terms of the strong field amplitudes by means of the appropriate projection operators. For reference we write the expressions for the quantities of principal interest:

a) Hydrogen or Tritium Atoms

$$\langle\sigma_z\rangle = |b_1|^2+|b_4|^2-|b_2|^2-|b_3|^2$$
$$\langle\sigma_x\rangle = 2\mathrm{Re}(b_1^* b_2+b_4^* b_3) \quad (20)$$
$$\langle\sigma_y\rangle = 2\,\mathrm{Im}(b_1^* b_2+b_4^* b_3)$$

b) Deuterium Atoms

$$\langle S_z\rangle = P_3 = |b_1|^2+|b_6|^2-|b_3|^2-|b_4|^2$$
$$3\langle S_z\rangle^2-2 = P_{33} = |b_1|^2+|b_6|^2+|b_3|^2+|b_4|^2 - 2|b_2|^2-2|b_5|^2 \quad (21)$$
$$\langle S_x\rangle = \sqrt{2}\,\mathrm{Re}(b_1^* b_2+b_2^* b_3+b_5^* b_4+b_6^* b_5)$$
$$\langle S_y\rangle = \sqrt{2}\,\mathrm{Im}(b_1^* b_2+b_2^* b_3+b_5^* b_4+b_6^* b_5)$$

where all expectation values refer to nuclear polarization. Similar expressions may be written for electronic polarization. It is clear that we may use these expressions to calculate the polarization parameters in either the initial coordinate system (unprimed amplitudes), or in the rotated coordinate system (primed amplitudes), depending on the desired reference axes.

TABLE II

POLARIZATION IN INTERMEDIATE FIELDS

Hydrogen or Tritium Atoms

State	P(nuclear)	P(electronic)
1	1	1
2	$-\delta$	δ
3	-1	-1
4	δ	$-\delta$

Deuterium Atoms

State	P_3(nuclear)	P_{33}(nuclear)	P(electronic)
1	1	1	1
2	$\frac{1}{2}(1-\delta_+)$	$-\frac{1}{2}(1+3\delta_+)$	δ_+
3	$-\frac{1}{2}(1+\delta_-)$	$-\frac{1}{2}(1-3\delta_-)$	δ_-
4	-1	1	-1
5	$-\frac{1}{2}(1-\delta_-)$	$-\frac{1}{2}(1+3\delta_-)$	$-\delta_-$
6	$\frac{1}{2}(1+\delta_+)$	$-\frac{1}{2}(1-3\delta_+)$	$-\delta_+$

The equations of motion of the probability amplitudes (Eqs. 8 and 9) may be solved in a straightforward way if the field is assumed to be constant and if the (negligible) nuclear terms are omitted. We present these solutions here primarily because they are useful in understanding and describing the nature of the more general solutions.

If we neglect the nuclear term in the Hamiltonian, the differential equations for the hydrogen or tritium atom become

$$\begin{aligned} i\dot{b}_1 &= \tfrac{1}{2}(x+\tfrac{1}{2})\omega b_1 \\ i\dot{b}_2 &= \tfrac{1}{2}(x-\tfrac{1}{2})\omega b_2 + \tfrac{1}{2}\omega b_4 \\ i\dot{b}_3 &= \tfrac{1}{2}(-x+\tfrac{1}{2})\omega b_3 \\ i\dot{b}_4 &= \tfrac{1}{2}\omega b_2 - \tfrac{1}{2}(\tfrac{1}{2}+x)\omega b_4 \quad , \end{aligned} \tag{22}$$

where the z axis is defined by the (constant) magnetic field direction, $x = B/B_o$, and $\omega = \Delta W/\hbar$. If the initial conditions are $b_1 = \varepsilon_1$, $b_2 = \varepsilon_2$, $b_3 = \varepsilon_3$, and $b_4 = \varepsilon_4$, the general solution may be written

$$\begin{aligned} b_1 &= \varepsilon_1 \exp[-i(\tfrac{1}{2}+x)\tfrac{1}{2}\omega t] \\ b_2 &= \tfrac{1}{2}\left\{\varepsilon_2(1-x/\beta)-\varepsilon_4(1/\beta)\right\}\exp[i(\tfrac{1}{2}+\beta)\tfrac{1}{2}\omega t] \\ &\quad +\tfrac{1}{2}\left\{\varepsilon_2(1+x/\beta)+\varepsilon_4(1/\beta)\right\}\exp[i(\tfrac{1}{2}-\beta)\tfrac{1}{2}\omega t] \\ b_3 &= \varepsilon_3 \exp[-i(\tfrac{1}{2}-x)\tfrac{1}{2}\omega t] \\ b_4 &= \tfrac{1}{2}\left\{-\varepsilon_2(1/\beta)+\varepsilon_4(1+x/\beta)\right\}\exp[i(\tfrac{1}{2}+\beta)\tfrac{1}{2}\omega t] \\ &\quad +\tfrac{1}{2}\left\{\varepsilon_2(1/\beta)+\varepsilon_4(1-x/\beta)\right\}\exp[i(\tfrac{1}{2}-\beta)\tfrac{1}{2}\omega t] \quad , \end{aligned} \tag{23}$$

where $\beta = \sqrt{1+x^2}$. Only values of $\varepsilon_1 - \varepsilon_4$ for which $\varepsilon_1^2 + \varepsilon_2^2 + \varepsilon_3^2 + \varepsilon_4^2 = 1$ correspond to physical initial states.

Again neglecting the nuclear term in the Hamiltonian, the differential equations for the deuterium atom become

$$\begin{aligned} i\dot{b}_1 &= \tfrac{1}{2}(x+1)\omega b_1 \\ i\dot{b}_2 &= \tfrac{1}{2}\,x\,\omega b_2 + \frac{1}{\sqrt{2}}\,\omega b_6 \\ i\dot{b}_3 &= \tfrac{1}{2}(x-1)\omega b_3 + \frac{1}{\sqrt{2}}\,\omega b_5 \\ i\dot{b}_4 &= \tfrac{1}{2}(-x+1)\omega b_4 \\ i\dot{b}_5 &= \frac{1}{\sqrt{2}}\,\omega b_3 - \tfrac{1}{2}\,x\,\omega b_5 \\ i\dot{b}_6 &= \frac{1}{\sqrt{2}}\,\omega b_2 - \tfrac{1}{2}(x+1)\omega b_6 \quad , \end{aligned} \tag{24}$$

where $x = B/B_o$, $\omega = 2\Delta W/(3\hbar)$, and again the z axis is defined by the magnetic field. The solutions may be written in terms of the initial vector ε as follows:

$$\begin{aligned} b_1 &= \varepsilon_1 \exp[-i(1+x)\tfrac{1}{2}\omega t] \\ b_2 &= \tfrac{1}{2}\left\{\varepsilon_2(1-[x+\tfrac{1}{2}]/\beta_+)-\varepsilon_6(\sqrt{2}/\beta_+)\right\}\exp[i(\tfrac{1}{2}+\beta_+)\tfrac{1}{2}\omega t] \\ &\quad +\tfrac{1}{2}\left\{\varepsilon_2(1+[x+\tfrac{1}{2}]/\beta_+)+\varepsilon_6(\sqrt{2}/\beta_+)\right\}\exp[i(\tfrac{1}{2}-\beta_+)\tfrac{1}{2}\omega t] \\ b_3 &= \tfrac{1}{2}\left\{\varepsilon_3(1-[x-\tfrac{1}{2}]/\beta_-)-\varepsilon_5(\sqrt{2}/\beta_-)\right\}\exp[i(\tfrac{1}{2}+\beta_-)\tfrac{1}{2}\omega t] \\ &\quad +\tfrac{1}{2}\left\{\varepsilon_3(1+[x-\tfrac{1}{2}]/\beta_-)+\varepsilon_5(\sqrt{2}/\beta_-)\right\}\exp[i(\tfrac{1}{2}-\beta_-)\tfrac{1}{2}\omega t] \\ b_4 &= \varepsilon_4 \exp[-i(1-x)\tfrac{1}{2}\omega t] \\ b_5 &= \tfrac{1}{2}\left\{-\varepsilon_3(\sqrt{2}/\beta_-)+\varepsilon_5(1+[x-\tfrac{1}{2}]/\beta_-)\right\}\exp[i(\tfrac{1}{2}+\beta_-)\tfrac{1}{2}\omega t] \\ &\quad +\tfrac{1}{2}\left\{\varepsilon_3(\sqrt{2}/\beta_-)+\varepsilon_5(1-[x-\tfrac{1}{2}]/\beta_-)\right\}\exp[i(\tfrac{1}{2}-\beta_-)\tfrac{1}{2}\omega t] \\ b_6 &= \tfrac{1}{2}\left\{-\varepsilon_2(\sqrt{2}/\beta_+)+\varepsilon_6(1+[x+\tfrac{1}{2}]/\beta_+)\right\}\exp[i(\tfrac{1}{2}+\beta_+)\tfrac{1}{2}\omega t] \\ &\quad +\tfrac{1}{2}\left\{\varepsilon_2(\sqrt{2}/\beta_+)+\varepsilon_6(1-[x+\tfrac{1}{2}]/\beta_+)\right\}\exp[i(\tfrac{1}{2}-\beta_+)\tfrac{1}{2}\omega t] \quad , \end{aligned} \tag{25}$$

where $\beta_\pm = \sqrt{x^2 \pm x + 9/4}$. Only those values of $\varepsilon_1 - \varepsilon_6$ for which $\varepsilon_1^2 + \varepsilon_2^2 + \varepsilon_3^2 + \varepsilon_4^2 + \varepsilon_5^2 + \varepsilon_6^2 = 1$ correspond to physical initial states.

3. APPLICATIONS

We will consider several applications of the theory just described, all of which are of interest in the design and utilization of polarized-ion sources. For the most part, where numerical results are presented, we will have in mind polarized-ion sources of the Lamb-shift type. We will consider the following problems:

a) "Adiabatic reduction" of a large (longitudinal) to a small (longitudinal) magnetic field;

b) Adiabatic reduction of a large (longitudinal) to a small (transverse) magnetic field;

c) The sudden zero field crossing technique of polarization enhancement;

d) Depolarization effects associated with the addition of two electrons to a polarized H^+ or D^+ ion beam.

We first make some general observations about the conditions required for adiabaticity. At low fields a one-electron atom in a pure state will behave like an elementary particle which has the magnetic moment of the electron but the total spin angular momentum of the atom. Since a free electron precesses about a field at the rate of $\mu_o g_J/h$ = 2.8 MHz/G, a hydrogen atom in the F = 1 state

will precess at a rate of 1.4 MHz/G. (The pure F = 0 state has no polarization; thus, its precession rate, which would be infinite from this point of view, has no physical interpretation.) A deuterium atom in the F = 3/2 state will precess at 0.93 MHz/G while one in an F = 1/2 state will precess at 2.8 MHz/G. Thus, for low fields, transitions will be induced only if the field direction changes rapidly with respect to the appropriate one of these precession frequencies. We will adopt the term "critical frequency" to denote the particular precession frequency which serves as the boundary between the zero transition (adiabatic) region and the complete transition (diabatic) region.

At high fields the critical frequency is directly related to the hyperfine splitting. To illustrate the connection, we consider a hydrogen atom which has, at zero time, its electron spin aligned with the magnetic field (+z-axis) and its proton spin aligned with the +x-axis. In terms of the solutions given in Section 2, the initial conditions which represent this situation are $\epsilon_1 = \epsilon_2 = 1/\sqrt{2}$ and $\epsilon_3 = \epsilon_4 = 0$. From Eqs. 20 and 23, we find that

$$\langle \sigma_x \rangle = 2\mathrm{Re}(b_1^* b_2 + b_4^* b_3) \overset{x\to\infty}{\to} \cos(\Delta W/2\hbar)t. \quad (26)$$

Thus, if the field is sufficiently strong to maintain the alignment of the electron, i.e., for $x \gg 1$, the component of the proton spin angular momentum which is not parallel to B will precess around the magnetic field at one-half of the hyperfine frequency. The classical picture that is involved is as follows. Neglecting, as in Eqs. 22 and 24, the $\mu_N \cdot B$ term in the Hamiltonian, we may say that the electron precesses about the applied magnetic field with a frequency corresponding to the free-electron precession rate, while the nucleus precesses about the electron with a frequency closely related to the normal hyperfine splitting. If the external field is to be changed in an adiabatic manner, it must be changed slowly with respect to both frequencies. At low fields the critical frequency therefore approaches the electron precession frequency (modified by the total angular momentum of the atom) while at high fields it approaches one-half of the normal hyperfine frequency.

For both the low- and high-field regions, the critical frequencies arrived at, in this semiclassical picture, correspond exactly to the energy separation between the initial state and the nearest neighboring state. For intermediate field strengths the motion is complicated; the electron and proton may be said to "tumble" about each other. However, from the form of Eq. 26 it is clear that the separation between the initial and the adjacent state still corresponds to the critical frequency (see Fig. 3).

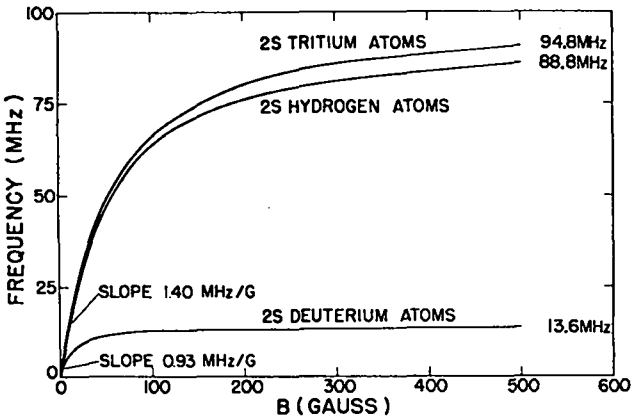

Fig. 3. Plot of the critical frequency for 2S tritium, hydrogen, and deuterium atoms versus magnetic field strength. For 1S atoms both the horizontal and vertical scales should be multiplied by 8.

For deuterium atoms we obtain similar results. For an atom which has, at zero time, the electron aligned with the field (+z-axis) and the deuteron in an $m_I = 1$ state with respect to the +x-axis, the appropriate initial conditions are $\epsilon_1 = \epsilon_3 = 1/2$, $\epsilon_2 = 1/\sqrt{2}$, and $\epsilon_4 = \epsilon_5 = \epsilon_6 = 0$. From Eqs. 21 and 25, we find that

$$\langle S_x \rangle = \sqrt{2}\,\mathrm{Re}(b_1^* b_2 + b_2^* b_3 + b_5^* b_4 + b_6^* b_5) \overset{x\to\infty}{\to} \cos(\Delta W/3\hbar)t\,. \quad (27)$$

In this case the high-field critical frequency is one-third of the hyperfine frequency. However, we note that the critical frequency again corresponds to the energy separation between the initial and the adjacent state (see Fig. 3).

Adiabatic Reduction of a Large (Longitudinal) to a Small (Longitudinal) Magnetic Field

Maxwell's equations imply the following (first order) relation between the radial and axial components of a cylindrically symmetric magnetic field:

$$B_r = -\frac{r}{2}\frac{\partial B_z}{\partial z}\,. \quad (28)$$

Thus, except at r = 0, a changing magnetic field strength B_z is always accompanied by a radial field component. The angle between the field direction and the z-axis is therefore given by

$$\tan \theta = \frac{B_r}{B_z} = - \frac{r}{2B_z} \frac{\partial B_z}{\partial z} . \qquad (29)$$

For example, if we have a uniformly falling field ($B_z = - cz$), Eq. 29 becomes

$$\tan \theta = \frac{r}{2z} = \frac{r}{2vt} , \qquad (30)$$

where z = vt for a beam moving with velocity v. The same result holds for an exponentially falling field ($B_z = ce^{-z/Z}$). Thus, except at r = 0, for any kind of declining field, there will be a changing field direction; it is this rate of change that must be kept small with respect to the relevant critical precession frequency. For a linearly falling field, this angular rate of change is

$$\omega = \frac{d}{dt} \left(\tan^{-1} \frac{r}{2vt}\right) = \frac{-(r/2v)}{(r/2v)^2+t^2} . \qquad (31)$$

Except at small t (and therefore small B) the rate of rotation is inversely proportional to r. Thus, the outer region of a large beam will be less subject to depolarization than the inner region.

We now consider the depolarization effects for some particular field shapes. (These results were obtained with the computer code given in the Appendix.) Figure 4 presents some numerical results for a field which falls from an initial value of 575 G to a final value of 5 G with an exponential law: $B_z = 575\ e^{-z/Z} + 5$. (The particular velocity of 30 cm/μsec, which is that used in a Lamb-shift polarized-ion source, is assumed for all numerical results presented in this report.) Particles traveling on the axis (r = 0) experience no change in field direction and hence undergo no transitions. In each case we plot the retained fraction of the atoms; that is, the fraction which does not make a transition to any other quantum state.

Figure 5 presents curves similar to those of Fig. 4 for a particular magnetic field configuration approximating that which may be obtained by a solenoid in an iron cylinder with a small oppositely directed correction current about one diameter from the main solenoid end. (The exact field shape used is shown in Fig. 6.) The depolarization effects for

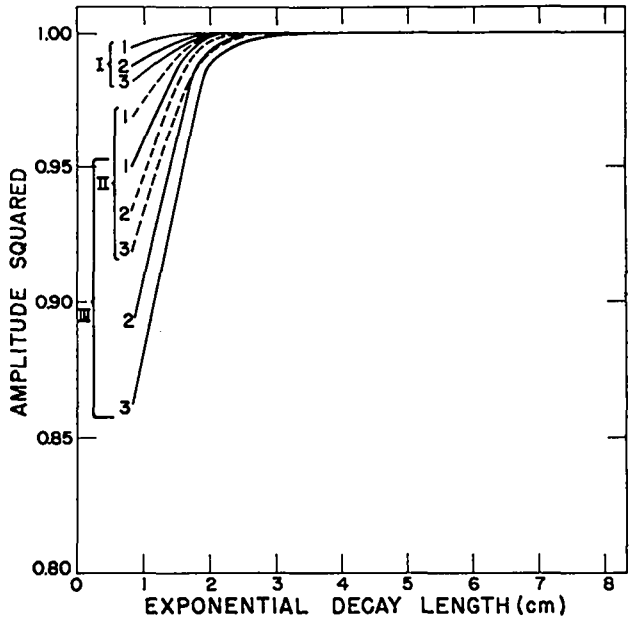

Fig. 4. Retained fraction of hydrogen atoms in state 1 (I), deuterium atoms in state 1 (II), and deuterium atoms in state 2 (III) for an exponentially shaped field which decays from 575 to 5 G. The abscissa is the "1/e" length Z. The curves marked 1, 2, and 3 correspond to particles which travel 1.25, 2.50, and 3.75 cm from the axis. A velocity of 30 cm/μsec is assumed.

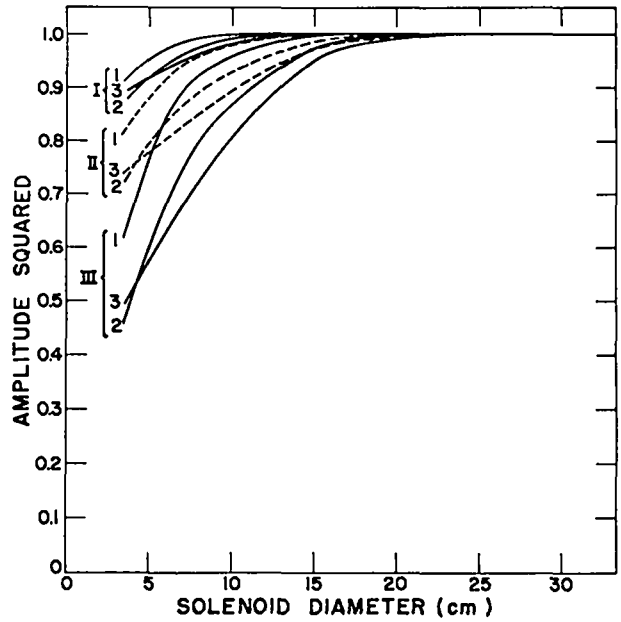

Fig. 5. Retained fraction of hydrogen atoms in state 1 (I), deuterium atoms in state 1 (II), and deuterium atoms in state 2 (III) for a particular axial field shape which can achieved with a shielded solenoid (see Fig. 6). Curves are labeled as in Fig. 4. The abscissa refers to the diameter of the solenoid shield. A velocity of 30 cm/μsec is assumed.

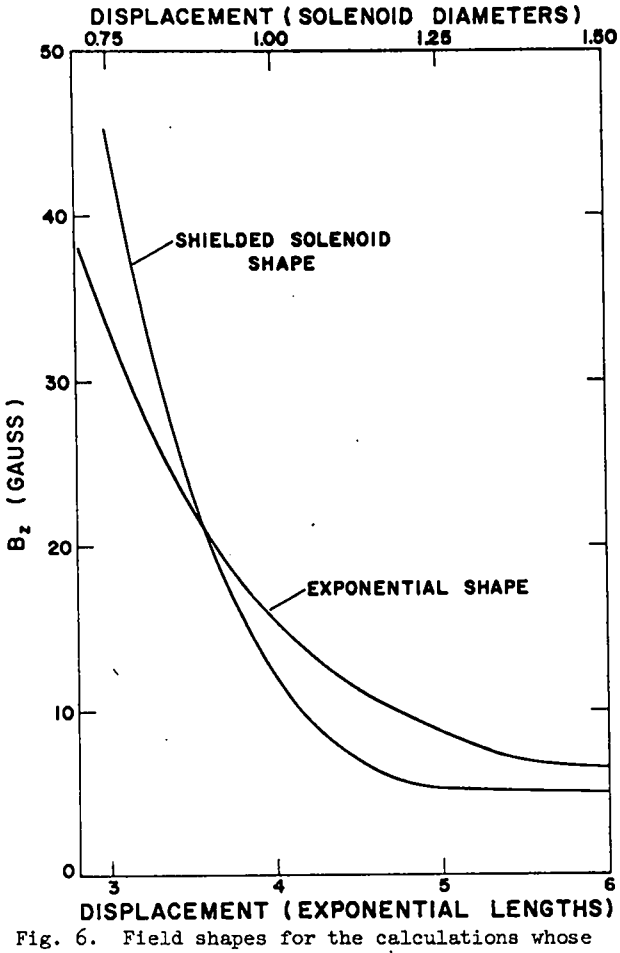

Fig. 6. Field shapes for the calculations whose results are presented in Figs. 4 and 5.

a field of this general shape are somewhat larger than with the exponential field. This points out that the exponential shape is nearly ideal, since B_z changes more and more slowly as the (more critical) lower field levels are reached.

Adiabatic Reduction of a Large (Longitudinal) to a Small (Transverse) Field

Figure 7 presents the retained fraction for an exponentially declining axial field and a transverse final field direction; that is, the field on the axis, in gauss, is described by $B_z = 575\ e^{-z/Z}$, $B_x = 5$. It is somewhat easier to induce depolarization in this case than in the case where the final field is longitudinal, because θ ($= \tan^{-1} B_r/B_z$) must change by 90°, whereas for a longitudinal final field, θ increases to some maximum value and then returns to zero. The critical region is where $B_x = B_z$, since the field rotation rate is maximum there. The maximum allowable ω is determined by the total magnetic field B ($= \sqrt{B_x^2 + B_y^2 + B_z^2}$). The details of

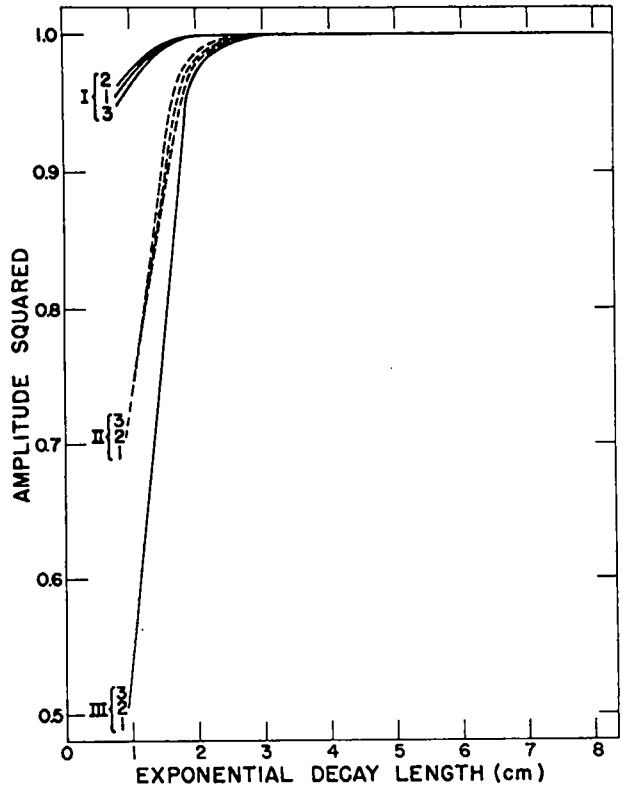

Fig. 7. Retained fraction of hydrogen atoms in state 1 (I), deuterium atoms in state 1 (II), and deuterium atoms in state 2 (III) for an exponentially declining axial field and a transverse final field. The curves and the abscissa are labeled as in Fig. 4. A velocity of 30 cm/μsec is assumed.

the shape of the B_x field are apparently unimportant so long as B_x has risen to its full value before B_z drops below one or two times the final B_x value.

Figure 8 shows the retained fraction for a final transverse field of 5 G ($B_x = 5$) and for a longitudinal field 5 G less than that plotted in Fig. 6. (The axial field approaches zero for large displacement.) Again the depolarization effects are more severe in this case than in the exponential one. This is because the rate of fall of the axial field in the critical region (near 5 G) is greater in the present case.

From Figs. 4, 5, 7, and 8, it is seen that, of the states considered, state-1 hydrogen atoms are depolarized the least, while state-2 deuterium atoms are depolarized the most. On the basis of the critical-frequency arguments, we expect hydrogen atoms to be less subject to depolarization than deuterium atoms (in agreement with the calculations). However, these arguments do not account for the difference between state-1 and state-2 deuterium

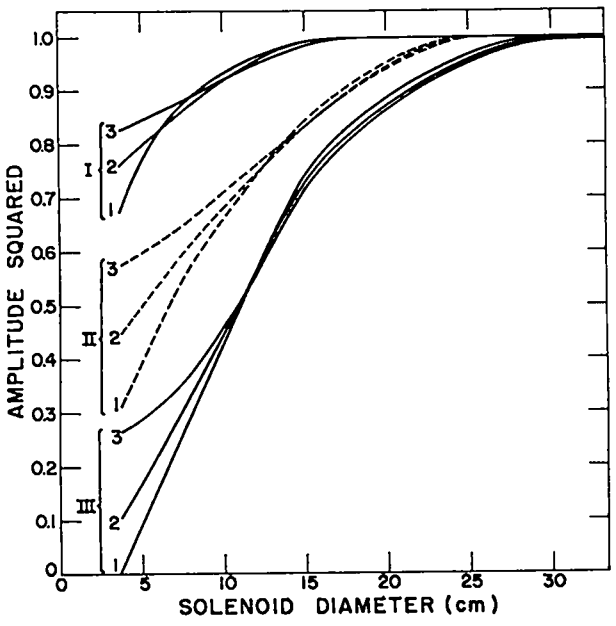

Fig. 8. Retained fraction of hydrogen atoms in state 1 (I), deuterium atoms in state 1 (II), and deuterium atoms in state 2 (III) for a particular axial field shape (see text) and a transverse final field. The curves and the abscissa are labeled as in Fig. 5. A velocity of 30 cm/μsec is assumed.

atoms. Possibly state-2 deuterium atoms are more readily depolarized than state-1 atoms because there are two nearby states instead of one to which transitions may occur.

A transverse field destroys cylindrical symmetry, so that particles at a given radius, but at different azimuthal angle with respect to the beam axis, will undergo different field rotations. Thus, atoms in different parts of a beam will be subject to different transition probabilities. This is, of course, not important if the transition probabilities are all kept near zero. The curves presented in Figs. 7 and 8 assume an average situation; i.e., they correspond to a ray in the y-z plane and to a final transverse field in the x-direction.

Sudden Zero Field Crossing Technique of Polarization Enhancement

It has been suggested by Sona[3] that it should be possible to enhance the polarization of a metastable H or D beam with the aid of a sudden reversal of the magnetic field direction. In this scheme the magnetic field is first reduced adiabatically to a low level; e.g., ∿1 G. Then a sudden reversal to ∿ -1 G takes place. If the reversal is so sudden that the atoms cannot follow it, the states become, with respect to the new magnetic field direction, different quantum states as follows:

Hydrogen	Deuterium
1 → 4	1 → 4
2 → 2	2 → 3
3 → 1	3 → 2
4 → 4	4 → 1
	5 → 6
	6 → 5

Thus, for hydrogen atoms, if one starts at high positive fields with an equal mixture of states 1 and 2 (0% polarization), after a sudden zero crossing followed by an adiabatic increase to a high negative field, one obtains an equal mixture of states 2 and 3 (100% polarization). For deuterium atoms, if at high positive fields we have an equal mixture of states 1, 2, and 3 ($P_3 = P_{33} = 0$), a sudden zero crossing followed by an adiabatic increase to a large negative field leads to an equal mixture of the states 2, 3, and 4 ($P_3 = -2/3$, $P_{33} = 0$). This process has been applied with good results at two laboratories.[4,5]

Our concern here is the extent to which one can achieve these diabatic transitions for practical beam sizes and magnetic field shapes. Our attention will be focussed mainly on hydrogen or deuterium atoms in their 1-states. [For hydrogen there is no difference between state 2 for a very small positive and a very small negative field, so it is not meaningful to inquire whether the atom "followed" the field direction or not. For deuterium atoms in states 2 and 3, such a question is meaningful, but since equal initial populations of 2 and 3 are involved in the applications we have in mind, symmetrical transitions (or the lack thereof) between them are of no consequence.]

Consider again the uniformly falling field for which $B_z = -cz = -cvt$ and $B_r = \frac{1}{2}cr$. At $z = 0$ the (minimum) field is $B = \frac{1}{2}cr$. The field angular roration rate is, again,

$$\omega = \frac{-(r/2v)}{(r/2v)^2+t^2} \quad . \tag{32}$$

Note that this frequency is independent of c, the rate of fall of the B_z field. However, the minimum field, for given r, is proportional to c. Thus, increasing the rate of fall of B_z has the net effect of raising the minimum field and thus the ability of the atom to follow the field reversal is improved. Larger r increases both the minimum

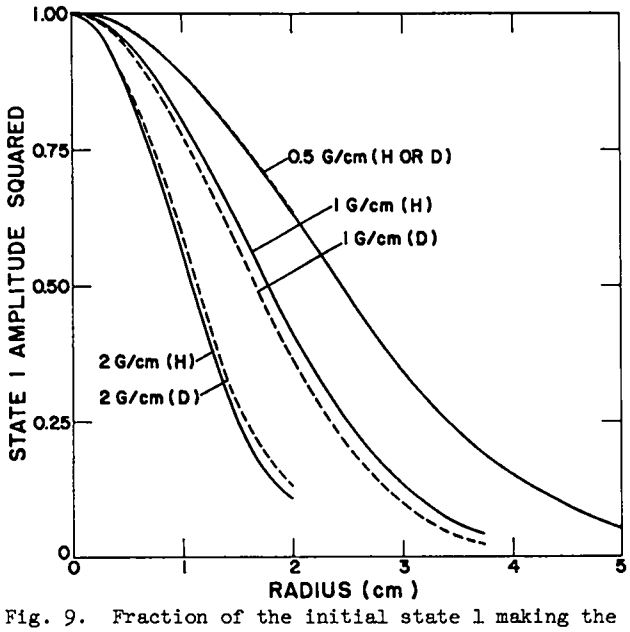

Fig. 9. Fraction of the initial state 1 making the desired transition when the field is linearly reversed at the indicated rate. The abscissa is the radius with respect to the (cylindrically symmetric) field axis. Slightly different results are obtained for hydrogen state 1 (H) and deuterium state 1 (D), as indicated. A velocity of 30 cm/μsec is assumed.

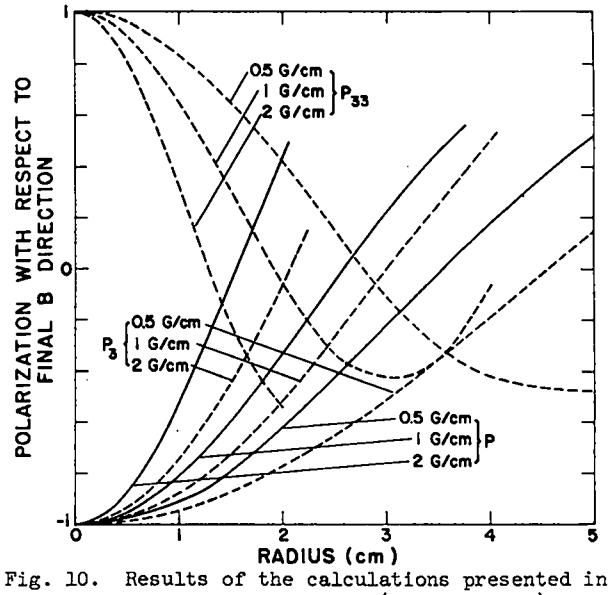

Fig. 10. Results of the calculations presented in Fig. 9 expressed in terms of P (for hydrogen) and P_3 and P_{33} (for deuterium). The polarizations are expressed with respect to the final field direction. A velocity of 30 cm/μsec is assumed.

field and decreases the angular rate with which the field reverses, and thus also improves the ability of the atom to follow the reversal. From this discussion it appears that 1) the field must reverse as slowly as possible (contrary to one's first impression) and 2) there exists a maximum beam diameter, for a given rate of fall for B_z, for which the scheme will be applicable. As pointed out by Sona,[3] the presence of transverse (stray) field components will place a lower limit on the field parameter c.

Figure 9 shows the fraction of the initial state 1 making transitions to state 3 for hydrogen or to state 4 for deuterium atoms, as a function of beam radius for several rates of fall for B_z. There is no appreciable difference between the results for hydrogen and deuterium. A priori, one would expect a larger fraction of the deuterium atoms to make transitions since the relevant precession frequency (with respect to which the field must rotate rapidly) is only two-thirds as large for deuterium as it is for hydrogen. The deviation from expectations is probably because, at a given (low) magnetic field, the deuterium atom is less well-described as a simple particle (with spin 3/2) than is the hydrogen atom (with spin 1).

Figure 10 presents the information given in Fig. 9 in terms of polarization versus beam radius. For hydrogen atoms this presentation carries no new information, but for deuterium atoms, one wishes to know of the effect on both vector and tensor polarization. It would be equivalent, for our purposes, to specify the relative population of each of the final states other than the initial state.

Depolarization Effects Associated with the Addition of Two Electrons to a Polarized H^+ or D^+ Ion Beam

If a positive H or D ion has two electrons added to it in a gas or foil, there may be a time interval during which the system is a neutral atom. During this time some depolarization will take place if a) the time interval is long enough and b) the magnetic field in the stripper region is small or zero; i.e., unless $x \gg 1$. Similar arguments apply to the case of the stripping of two electrons by a negative ion. This point will be further discussed later.

Let us assume that the magnetic field, if any, in the "adder" region is constant. We choose our z-axis to be parallel with the field. The nuclear polarization may be parallel to the z-axis or inclined at some angle with respect to it. (The solutions presented in Section 2 are sufficiently

general to handle any such orientation.)

First, we consider hydrogen ions with the nuclear spin parallel to the stripper field. If we assume that the first electron is captured into the ground state, the atom will be in either state 1 or in state 4 (equal probability), where we refer to strong field states regardless of the actual field strength. From the general solutions already given, atoms which are in state 1 initially will remain so; thus, for these atoms, we have

$$\langle\sigma_z\rangle = 1 \ . \tag{33}$$

The time dependence of $\langle\sigma_z\rangle$ for an atom initially in state 4 is obtained from the general solution (Eq. 23) with $\varepsilon_1 = \varepsilon_2 = \varepsilon_3 = 0$ and $\varepsilon_4 = 1$:

$$\langle\sigma_z\rangle = \frac{1}{x^2+1}\left(x^2+\cos\sqrt{1+x^2}\,\frac{\Delta W}{\hbar}\,t\right) \ ; \tag{34}$$

i.e., for $x = 0$ depolarization occurs with the normal hyperfine frequency $\Delta W/\hbar$ as the characteristic rate. If the time interval (τ) between the pick-up of the first and of the second electron is random, and long compared to $\hbar/\Delta W$, then, for a beam of particles, $\langle\sigma_z\rangle$ will have the average value $x^2/(x^2+1)$. Combining Eqs. 33 and 34 we obtain for the overall beam polarization

$$P = \tfrac{1}{2}[1+x^2/(x^2+1)] \qquad (\hbar/\Delta W \ll \tau) \ . \tag{35}$$

If the time τ is sufficiently short, no depolarization occurs. For zero magnetic field ($x = 0$), we see that a maximum overall depolarization of 50% may occur; for large fields ($x \gg 1$), no depolarization will occur. Consideration of the case where the initial nuclear polarization and stripper field are antiparallel gives, except for overall sign, a result identical to that given above. That is, for an atom initially in state 3

$$\langle\sigma_z\rangle = -1 \ , \tag{36}$$

while for an atom initially in state 2

$$\langle\sigma_z\rangle = -\frac{1}{x^2+1}\left(x^2+\cos\sqrt{1+x^2}\,\frac{\Delta W}{\hbar}\,t\right) \ . \tag{37}$$

Thus, the overall polarization for an equal mixture of states 2 and 3 may be written

$$P = -\tfrac{1}{2}[1+x^2/(x^2+1)] \qquad (\hbar/\Delta W \ll \tau) \ . \tag{38}$$

In summary, if depolarization is to be avoided, either the time between the first and second collisions must be small compared to $\hbar/\Delta W$ or a large magnetic field must be present.

If the nuclear spin is perpendicular to the adder magnetic field direction (z-axis), the (equally probably) initial states are as follows: for the electron spin parallel to z, $\langle\sigma_x\rangle = 1$ implies $\varepsilon_1 = \varepsilon_2 = 1/\sqrt{2}$ and $\varepsilon_3 = \varepsilon_4 = 0$; if the electron spin is antiparallel to z, $\langle\sigma_x\rangle = 1$ implies $\varepsilon_1 = \varepsilon_2 = 0$ and $\varepsilon_3 = \varepsilon_4 = 1/\sqrt{2}$. For the first of these initial conditions we obtain

$$\langle\sigma_x\rangle = \tfrac{1}{2}(1-x/\beta)\cos\left[(1+x+\beta)\frac{\Delta W}{2\hbar}\,t\right]+\tfrac{1}{2}(1+x/\beta) \times\cos\left[(1+x-\beta)\frac{\Delta W}{2\hbar}\,t\right] \ , \tag{39}$$

where $\beta = (1+x^2)^{\frac{1}{2}}$. For the second initial condition we obtain

$$\langle\sigma_x\rangle = \tfrac{1}{2}(1+x/\beta)\cos\left[(1-x+\beta)\frac{\Delta W}{2\hbar}\,t\right]+\tfrac{1}{2}(1-x/\beta) \times\cos\left[1-x-\beta)\frac{\Delta W}{2\hbar}\,t\right] \ . \tag{40}$$

For very large x, Eqs. 39 and 40 each become

$$\langle\sigma_x\rangle \overset{x\to\infty}{\to} \cos\frac{\Delta W}{2\hbar}\,t \ ; \tag{41}$$

i.e., the polarization precesses at the expected high field rate. For small fields Eqs. 39 and 40 each become

$$\langle\sigma_x\rangle \overset{x\to 0}{\to} \tfrac{1}{2}\left(1+\cos\frac{\Delta W}{\hbar}\,t\right) \ ; \tag{42}$$

i.e., again depolarization occurs with the normal hyperfine frequency as the characteristic rate. (The zero field limit must, of course, be independent of the direction of the assumed angle between the nuclear polarization and the magnetic field.) A more general orientation of the magnetic field axis may be considered with the aid of the solutions given in Section 2.

For deuterons the situation is similar but slightly more complicated. The vector and tensor polarization P_3 and P_{33} for each of the (strong field) initial states 1-6 is as follows:

Initial State	P_3	P_{33}
1	1	1
2	$\frac{1}{\beta_+^2}[1-\cos(\frac{2\Delta W}{3\hbar})\beta_+ t]$	$-\frac{1}{\beta_+^2}[2x^2+2x+3/2+3\cos(\frac{2\Delta W}{3\hbar})\beta_+ t]$
3	$-\frac{1}{\beta_-^2}[x^2-x+5/4+\cos(\frac{2\Delta W}{3\hbar})\beta_- t]$	$\frac{1}{\beta_-^2}[x^2-x-3/4+3\cos(\frac{2\Delta W}{3\hbar})\beta_- t]$
4	-1	1
5	$-\frac{1}{\beta_-^2}[1-\cos(\frac{2\Delta W}{3\hbar})\beta_- t]$	$-\frac{1}{\beta_-^2}[2x^2-2x+3/2+3\cos(\frac{2\Delta W}{3\hbar})\beta_- t]$
6	$\frac{1}{\beta_+^2}[x^2+x+5/4+\cos(\frac{2\Delta W}{3\hbar})\beta_+ t]$	$\frac{1}{\beta_+^2}[x^2+x-3/4+3\cos(\frac{2\Delta W}{3\hbar})\beta_+ t]$,

(43)

where $\beta\pm = (x^2 \pm x + 9/4)^{\frac{1}{2}}$. We note that, at zero field, the time dependence becomes of the form $\cos(\Delta W/\hbar)t$, so once again depolarization occurs at the normal hyperfine frequency.

For a deuteron beam initially in the $m_I = 1$ state with respect to the adder field direction, strong field states 1 and 6 are populated with equal probability; the time-averaged polarization parameters become

$$P_3 = \tfrac{1}{2}(1+\frac{x^2-x+5/4}{x^2+x+9/4}) \qquad (\hbar/\Delta W \ll \tau) . \qquad (44)$$
$$P_{33} = \tfrac{1}{2}(1+\frac{x^2+x-3/4}{x^2+x+9/4})$$

Similarly, for $m_I = 0$ we obtain

$$P_3 = \tfrac{1}{2}[\frac{1}{x^2+x+9/4} - \frac{1}{x^2-x+9/4}] \qquad (\hbar/\Delta W \ll \tau) , \qquad (45)$$
$$P_{33} = -[\frac{x^2+x+3/4}{x^2+x+9/4} + \frac{x^2-x+3/4}{x^2-x+9/4}]$$

and, for $m_I = -1$

$$P_3 = -\tfrac{1}{2}[1+\frac{x^2-x+5/4}{x^2-x+9/4}] \qquad (\hbar/\Delta W \ll \tau) . \qquad (46)$$
$$P_{33} = \tfrac{1}{2}[1+\frac{x^2-x-3/4}{x^2-x+9/4}]$$

For $h/\Delta W \gg \tau$ no depolarization occurs. For zero field Eqs. 44-46 reduce to

m_I	P_3	P_{33}
1	7/9	1/3
0	0	-2/3
-1	-7/9	1/3

That is, the initial vector polarization is reduced to seven-ninths of its initial value while the initial tensor polarization is reduced to one-third of its initial value. We may summarize the zero field results as follows:

	Characteristic Frequency for Depolarization	Maximum Depolarization Vector	Maximum Depolarization Tensor
Protons	1420 MHz	1/2	--
Deuterons	327 MHz	2/9	2/3
Tritons	1517 MHz	1/2	--

In the above it is assumed that the intermediate atoms are formed in the ground state. At higher fields the depolarization is smaller; however, note that the characteristic frequency for depolarization becomes larger.

In the above discussion, it has been assumed that the first electron is added in the $1S_{1/2}$ state. However, the theory holds for capture into any J = 1/2 state, so long as the atom remains in this state until the second electron is added and provided that the appropriate hyperfine splitting is used in the description. If radiative decay occurs, some additional depolarization will result. On the other hand, relatively small magnetic fields will be sufficient to produce a strong field with respect to the higher hydrogen-atom excited states, and radiative decay in the presence of a strong field will result in no nuclear depolarization. Thus, a field strength which is sufficient to prevent depolarization of a $1S_{1/2}$ state is also sufficient to prevent depolarization while an atom is in an excited state

and during the decay of the atom (eventually to the $1S_{1/2}$ state).

For a "thick" adder, as required for a large negative ion yield, electrons may be added and subtracted several times before the particle escapes as a negative ion. The considerations above will apply to each time interval during which the particle exists as a neutral atom. For example, consider a proton which is converted to an H^- ion via the process $H^+ \rightarrow H^0 \rightarrow H^+ \rightarrow H^0 \rightarrow H^-$. If we assume zero magnetic field and that both of the time intervals during which the particle is neutral are large compared to $\hbar/\Delta W$, a depolarization of 75% (i.e. $1 - (\frac{1}{2})^2$) would be expected. For deuterons the vector depolarization would be $1 - (\frac{7}{9})^2$ and the tensor depolarization would be $1 - (\frac{1}{3})^2$. In practice, of course, both the number of charge exchange events and the interval between them will be random.

The stripping of two electrons from a negative ion presents a somewhat similar problem. However, a hydrogen negative ion has a diffuse wave function compared to a hydrogen atom. Thus, if one of the electrons is suddenly removed, the remaining electron will tend to be spread over a relatively large region. Stated differently, the atom will have a high probability of being produced in a state other than the ground state. Therefore, the effects discussed in the previous paragraph are expected to be more important in the stripping case than in the adding case. It is possible that studies of depolarization versus magnetic field could yield information about 1) the wave function of the hydrogen negative ion and 2) the nature of the collisions which induce radiative decay of the higher hydrogen atom states that are produced in the partial stripping of an H^- ion.

ACKNOWLEDGMENTS

It is a pleasure to thank Donald Dodder for a number of clarifying discussions. I also appreciate conversations with Bailey Donnally, Ralph Stevens, Joe McKibben, John Gammel, and Charles Drake.

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APPENDIX

A COMPUTER CODE FOR SOLVING THE ONE-ELECTRON SCHROEDINGER EQUATION

This code solves the time-dependent Schroedinger equation for a Hamiltonian of the form

$$\mathcal{H} = H_o + (\mu_o g_J \vec{J} + \mu_N g_I \vec{I}) \cdot B + a(\vec{I} \cdot \vec{J}) \ ,$$

where the notation is defined in the preceding pages. An arbitrary time dependence of the external magnetic field B is allowed. A numerical integration of the resulting set of linear first-order differential equations is carried out with automatic error control.

The input for the code is as follows:

Card 1 — FORMAT (I6)

- NZ — number of points at which axial and radial field table is to be specified
  - = 0 if no table to be specified

Card 2 to Card (NZ + 1) — FORMAT (3F12.6)

- ZZ(I) — axial position (cm)
- BZZ(I) — axial field strength (G)
- BRR(I) — radial field strength 1 cm off axis (G)

CARD NZ + 2 — FORMAT (3I6)

- M — type of atom
  - = 1: for hydrogen atoms
  - = 2: for deuterium atoms
  - = 3: for tritium atoms
- NSTATE — initial state
  - = 1 to 4 if hydrogen or tritium atoms intermediate field states 1 to 4
  - = 1 to 6 if deuterium atom intermediate field states 1 to 6
  - = 11 to 14 if hydrogen or tritium strong field states 1 to 4
  - = 11 to 16 if deuterium atom strong field states 1 to 6
- MODE — option for defining magnetic field (see comments in BFIELD)
  - = 1: axial and radial fields as specified in table
  - = 2: axial field varies as a sine-squared function
  - = 3: axial field varies as an exponential function

Card NZ + 3 — FORMAT (3F12.6)

- TI — initial time (μsec)
- TTF — final time (μsec)
- HHP — time interval between output steps (μsec)

Card NZ + 4 — FORMAT (6F12.6)

- BZ1 — initial axial field (G)
- BZ2 — final axial field (G)
- BRMAX — final transverse field (G)
- Y1 — distance off axis (cm)
- PHI — azimuthal angle transverse field makes with respect to x axis (deg)
- VELOC — velocity of particle beam (cm/μsec)

Card NZ + 5

- Z1 — position at which axial field begins to decline or to be defined by table (cm)
- Z2 — position at which axial field assumes a constant final value (cm)
- Z3 — position at which transverse component begins to rise as sine-squared function (cm)
- Z4 — position at which transverse component assumes a constant final value (cm)

The code renormalizes the state vector to unity total probability before each print to remove accumulated normalization errors (via subroutine RENORM). If this error exceeds 1%, an error message is printed.

The time, field components and total field, nuclear polarization, electron polarization, and

squared amplitudes of the four (or six) strong field states are printed with reference to the coordinate system as defined by the user. These results are then printed a second time in terms of the intermediate field states with respect to a z axis defined by the instantaneous direction of the total field. In the second set of output the field is specified in terms of azimuthal and polar angles, and beam displacement is given instead of elapsed time.

The program consists of a main program MJRANA together with a number of subroutines. The function of each of the subroutines is briefly described below.

SUBROUTINE SETUPB

This subroutine reads in parameters necessary to specify the B field as described above. Certain often-used combinations of the input parameters are computed here.

SUBROUTINE BFIELD (T, BX, BY, BZ)

This subroutine computes the field components BX, BY, BZ at the time T, assuming Z = VELOC*T, X = 0, and Y = Y1.

SUBROUTINE DERIV (T, V, FD)

This subroutine computes the values of the first derivatives FD(I) (I = 1 to 8 or I = 1 to 12) given the value of T (time) and of the variables V(I) (I = 1 to 8 or I = 1 to 12). [Note that four (six) complex first-order differential equations result in eight (twelve) real first-order differential equations.]

SUBROUTINE PRINT (T, VS)

This subroutine prints the first type of output described above at the specified times and also stores the second type of output for later printing.

SUBROUTINE ROT (M, ALPHA, BETA, GAMMA, V)

This subroutine rotates the state vector V through the Euler angles α, β, and γ.

SUBROUTINE RENORM (N, V, VV)

This subroutine renormalizes the state vector V so that it has unity total length.

FUNCTION ARCTAN (Y, X)

This function computes arctangents, in degrees, for all zero and nonzero values of Y and X.

SUBROUTINE TABLE (Z, ZZ, NZ, I, MFLAG)

This subroutine performs a table look-up in the ordered table ZZ.

SUBROUTINE INTEG (NN, TI, TTF, HH, HHP, MM, VVM, IP, XO, TT, XXP)

This subroutine integrates an arbitrary system of real linear differential equations. The arguments of this subroutine are defined by comments in the main program listing. The monitoring feature (a periodic test of a specified variable against some limit) is not used. INTEG together with the subroutines START, RNGA, ACCRY, TEST, DIODE, ADAMS, and DOUBLE constitute the complete integration package.

```
      PROGRAM MJRANA(INPUT,OUTPUT,FILM,TAPE 12=FILM)                    MJRN0010
C  UNITS MICROSECONDS                                                   MJRN0011
      COMMON/BLOCK1/A1,A2,A3,A4,C1,RO                                   MJRN0012
      COMMON/BLOCK2/RSQ(6,201),TIME(201),BRX(201),BRY(201),BBZ(201),    MJRN0013
     1P3(201),P33(201),PEL(201),N,ITIME                                 MJRN0014
      COMMON/BLOCK3/M,NN                                                MJRN0015
      COMMON/BFLD/T1,T2,T3,T4,T5,T6,BZ1,BZ2,BRMAX,CPHI,SPHI,PI2,Y2,MODF,MJRN0016
     1VELOC                                                             MJRN0017
      COMMON/BFLDP/ZZ(100),BZZ(100),BRR(100),NZ                         MJRN0018
      DIMENSION XO(30),XXP(30),BPLOT(201)                               MJRN0019
      COMPLEX C1                                                        MJRN0020
    1 FORMAT(10I6)                                                      MJRN0021
    2 FORMAT(1H1)                                                       MJRN0022
    3 FORMAT(* PROTONS   *6F14.8)                                       MJRN0023
    4 FORMAT(* DEUTERONS *6F14.8)                                       MJRN0024
    5 FORMAT(* TRITONS   *6F14.8)                                       MJRN0025
    6 FORMAT(12F6.3)                                                    MJRN0026
    7 FORMAT(*      TIME        BX        BY        BZ         B        P3  MJRN0027
     1  P33       PEL         1         2         3         4         5    MJRN0028
     2 6*)                                                              MJRN0029
    8 FORMAT(14F9.4)                                                    MJRN0030
```

```
    9 FORMAT(6F12.6)                                                        MJRN0031
   10 FORMAT(* STRONG FIELD STATE COEFFICIENTS, INITIAL COORDINATE SYSTEMJRN0032
     1M*)                                                                   MJRN0033
   11 FORMAT(* INTERMEDIATE FIELD STATE COEFFICIENTS, COORDINATE SYSTEM MJRN0034
     1ROTATED SO NEW Z AXIS POINTS ALONG FIELD DIRECTION *)                 MJRN0035
   12 FORMAT(* P3=SQUARE, P33=PLUS, MAG FIELD PARAMS * 12F7.1)             MJRN0036
   13 FORMAT(* PARTICLE *I2,*  STATE *I2,* INITIAL STRONG FIELD COEFFS *MJRN0037
     1I2F6.3)                                                               MJRN0038
   15 FORMAT(*  Z(CM)       THETA       PHI         BZ          B        P3    MJRN0039
     1  P33       PFL         1         2         3         4         5       MJRN0040
     2 *)                                                                   MJRN0041
      READ 1,NZ                                                             MJRN0042
      IF(NZ.EQ.0) GO TO 100                                                 MJRN0043
      DO 90 I=1,NZ                                                          MJRN0044
      READ 9,ZZ(I),BZZ(I),BRR(I)                                            MJRN0045
   90 PRINT9,ZZ(I),BZZ(I),BRR(I)                                            MJRN0046
  100 ITIME=0                                                               MJRN0047
      PRINT 2                                                               MJRN0048
      READ 1,M,NSTATE,MODE                                                  MJRN0049
      PRINT 1,M,NSTATE,MODE                                                 MJRN0050
C  M=1,2, OR 3 FOR PROTONS,DEUTERONS, OR TRITONS                            MJRN0051
C  NSTATE= 1-4 OR 1-6 FOR INTERMEDIATE FIELD INITIAL STATES                 MJRN0052
C  NSTATE= 11-14 OR 11-16 FOR STRONG FIELD STATES                           MJRN0053
C  MODE=1,2, OR 3 DEPENDING ON BFIELD OPTION (SEE COMMENTS IN BFIELD)       MJRN0054
      READ 9,TI,TTF,HHP                                                     MJRN0055
      PRINT 9,TI,TTF,HHP                                                    MJRN0056
      CALL SETUPB                                                           MJRN0057
      CALL BFIELD(TI,BBX(1),BBY(1),BBZ(1))                                  MJRN0058
      HTOT=SQRT(BBX(1)**2+BBY(1)**2+BBZ(1)**2)                              MJRN0059
      ALPHA=0.0                                                             MJRN0060
      BETA=-(3.1415927/180.0)*ARCTAN(SQRT(BBX(1)**2+BBY(1)**2),BBZ(1))      MJRN0061
      GAMMA=-(3.1415927/180.0)*ARCTAN(BBY(1),BBX(1))                        MJRN0062
      DO 99 I=1,12                                                          MJRN0063
   99 X0(I)=0.0                                                             MJRN0064
      IF(M-2)101,102,103                                                    MJRN0065
  101 B0=63.448/1.001522                                                    MJRN0066
      A1=0.5*(1.0+0.001522/1.001522)                                        MJRN0067
      A2=0.5*(1.0-0.001522/1.001522)                                        MJRN0068
      A3=0.5*0.001522/1.001522                                              MJRN0069
      A4=0.0                                                                MJRN0070
      N=4                                                                   MJRN0071
      PRINT 3,A1,A2,A3,A4,B0                                                MJRN0072
      X=HTOT/63.448                                                         MJRN0073
   98 IF(NSTATE.GE.11) GO TO 164                                            MJRN0074
      DPLUS=SQRT(0.5+0.5*X/SQRT(1.0+X**2))                                  MJRN0075
      DMINUS=SQRT(0.5-0.5*X/SQRT(1.0+X**2))                                 MJRN0076
      GO TO (150,151,152,153),NSTATE                                        MJRN0077
  150 X0(1)=1.                                                              MJRN0078
      GO TO 104                                                             MJRN0079
  151 X0(3)=DPLUS                                                           MJRN0080
      X0(7)=DMINUS                                                          MJRN0081
      GO TO 104                                                             MJRN0082
  152 X0(5)=1.                                                              MJRN0083
      GO TO 104                                                             MJRN0084
  153 X0(3)=-DMINUS                                                         MJRN0085
      X0(7)=DPLUS                                                           MJRN0086
      GO TO 104                                                             MJRN0087
  154 NSTATE=NSTATE-10                                                      MJRN0088
      X0(2*NSTATE-1)=1.0                                                    MJRN0089
      GO TO 104                                                             MJRN0090
  102 B0=14.605/1.000233                                                    MJRN0091
      B0=(2.0/3.0)*B0                                                       MJRN0092
      A1=0.5+0.000233/1.000233                                              MJRN0093
      A2=0.5-0.000233/1.000233                                              MJRN0094
      A3=0.000233/1.000233                                                  MJRN0095
      A4=SQRT(0.5)                                                          MJRN0096
      N=6                                                                   MJRN0097
      PRINT 4,A1,A2,A3,A4,B0                                                MJRN0098
      X=HTOT/14.605                                                         MJRN0099
      IF(NSTATE.GE.11) GO TO 146                                            MJRN0100
      DPLUS=(X+1.0/3.0)/SQRT(1.0+2.0*X/3.0+X**2)                            MJRN0101
      DMINUS=(X-1.0/3.0)/SQRT(1.0-2.0*X/3.0+X**2)                           MJRN0102
```

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      GO TO (140,141,142,143,144,145),NSTATE                          MJRN0103
  140 XO(1)=1.0                                                       MJRN0104
      GO TO 104                                                       MJRN0105
  141 XO(3)=SQRT(0.5+0.5*DPLUS)                                       MJRN0106
      XO(11)=SQRT(0.5-0.5*DPLUS)                                      MJRN0107
      GO TO 104                                                       MJRN0108
  142 XO(5)=SQRT(0.5+0.5*DMINUS)                                      MJRN0109
      XO(9)=SQRT(0.5-0.5*DMINUS)                                      MJRN0110
      GO TO 104                                                       MJRN0111
  143 XO(7)=1.0                                                       MJRN0112
      GO TO 104                                                       MJRN0113
  144 XO(5)=-SQRT(0.5-0.5*DMINUS)                                     MJRN0114
      XO(9)=SQRT(0.5+0.5*DMINUS)                                      MJRN0115
      GO TO 104                                                       MJRN0116
  145 XO(3)=-SQRT(0.5-0.5*DPLUS)                                      MJRN0117
      XO(11)=SQRT(0.5+0.5*DPLUS)                                      MJRN0118
      GO TO 104                                                       MJRN0119
  146 NSTATE=NSTATE-10                                                MJRN0120
      XO(2*NSTATE-1)=1.0                                              MJRN0121
      GO TO 104                                                       MJRN0122
  103 BO=67.755/1.001623                                              MJRN0123
      A1=0.5*(1.0+0.001623/1.001623)                                  MJRN0124
      A2=0.5*(1.0-0.001623/1.001623)                                  MJRN0125
      A3=0.5*0.001623/1.001623                                        MJRN0126
      A4=0.0                                                          MJRN0127
      N=4                                                             MJRN0128
      PRINT 5,A1,A2,A3,A4,BO                                          MJRN0129
      X=BTOT/67.755                                                   MJRN0130
      GO TO 98                                                        MJRN0131
  104 ARG=2.0*3.1415927*1.401*2.00229                                 MJRN0132
      C1=CMPLX(0.0,-ARG)                                              MJRN0133
C  REFER INITIAL VECTOR TO PROBLEM DEFINED Z AXIS VIA APPROPRIATE ROTATIMJRN0134
      CALL ROT(N,ALPHA,BETA,GAMMA,XO)                                 MJRN0135
      NN=2*N                                                          MJRN0136
      PRINT 10                                                        MJRN0137
      PRINT 7                                                         MJRN0138
      CALL PRINT(TI,XO)                                               MJRN0139
      HH=0.0001                                                       MJRN0140
      MM=0                                                            MJRN0141
      VVM=0.0                                                         MJRN0142
      ABS=1.0E-05                                                     MJRN0143
      REL=1.0E-05                                                     MJRN0144
      CALL INTEG(NN,TI,TTF,HH,HHP,MM,VVM,ABS,REL,XO,TT,XXP)           MJRN0145
C   NN    NUMBER OF FIRST ORDER DIFFERENTIAL EQUATIONS                MJRN0146
C   TI    INITIAL VALUE OF INDEPENDENT VARIABLE                       MJRN0147
C   TTF   FINAL VALUE OF INDEPENDENT VARIABLE                         MJRN0148
C   HH    GUESS AT STEP SIZE                                          MJRN0149
C   HHP   PRINT STEP SIZE                                             MJRN0150
C   MM    INDEX OF VARIABLE TO BE MONITORED (0 IF NO MONITORING)      MJRN0151
C   VVM   VALUE TO MONITOR FOR                                        MJRN0152
C   ABS   MAXIMUM ACCEPTABLE ABSOLUTE ERROR IN ONE INTEGRATION STEP   MJRN0153
C   REL   MAXIMUM ACCEPTABLE RELATIVE ERROR IN ONE INTEGRATION STEP   MJRN0154
C   XO    VECTOR OF STARTING VALUES                                   MJRN0155
C   TT    VALUE OF INDEPENDENT VARIABLE RETURNED AT END OF INTEGRATION MJRN0156
C   XXP   VALUES OF DEPENDENT VARIABLES RETURNED AT END OF INTEGRATION MJRN0157
      PRINT 11                                                        MJRN0158
      PRINT 15                                                        MJRN0159
      NTIME=ITIME                                                     MJRN0160
      DO 110 I=1,NTIME                                                MJRN0161
      BTOT=SQRT(BBX(I)**2+BBY(I)**2+BBZ(I)**2)                        MJRN0162
      POSN=TIME(I)*VELOC                                              MJRN0163
      PHIF=ARCTAN(BBY(I),BBX(I))                                      MJRN0164
      THETAF=ARCTAN(SQRT(BBY(I)**2+BBX(I)**2),BBZ(I))                 MJRN0165
      PRINT 8,POSN,THETAF,PHIF,BBZ(I),BTOT,P3(I),P33(I),PEL(I),(BSQ(J,I)MJRN0166
     1,J=1,N)                                                         MJRN0167
  110 CONTINUE                                                        MJRN0168
C   THE FOLLOWING 18 CARDS PRODUCE A PLOT WITH LASL SUBROUTINES       MJRN0169
      CALL ADV(1)                                                     MJRN0170
      CALL DGA(50,950,50,800,TI,TTF,1.0,0.0)                          MJRN0171
      CALL DLNLN(10,10)                                               MJRN0172
      CALL SLLIN (10,01)                                              MJRN0173
      CALL SRLIN(10,02)                                               MJRN0174
```

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      DO 120 J=1,N                                                      MJRN0175
      DO 121 I=1,NTIME                                                  MJRN0176
  121 BPLOT(I)=BSQ(J,I)                                                 MJRN0177
  120 CALL PLOT(NTIME,TIME(1),1,BPLOT(1),1,44,1)                        MJRN0178
      CALL DGA(50,950,50,500,TI,TTF,1.0,-2.0)                           MJRN0179
      CALL SRLIN(6,01)                                                  MJRN0180
      CALL PLOT(NTIME,TIME(1),1,P33(1),1,16,0)                          MJRN0181
      CALL PLOT(NTIME,TIME(1),1,P3 (1),1,63,0)                          MJRN0182
      CALL LINCNT(60)                                                   MJRN0183
      PHI=PHI*180.0/3.1415927                                           MJRN0184
      WRITE(12,12)Z1,Z2,Z3,Z4,Z5,Z6,BZ1,BZ2,BRMAX,Y1,PHI,VELOC          MJRN0185
      WRITE(12,13)M,NSTATE,(XO(I),I=1,NN)                               MJRN0186
      CALL ADV(1)                                                       MJRN0187
      PRINT 13,M,NSTATE,(XO(I),I=1,NN)                                  MJRN0188
      GO TO 100                                                         MJRN0189
      END                                                               MJRN0190


      SUBROUTINE SETUPB                                                 SETB0010
C  READS IN FIELD PARAMETERS AND COMPUTES SOME FREQUENTLY USED QUAN-     SETB0011
C  TITIES FOR USE BY SUBROUTINE BFIELD                                   SETB0012
      COMMON/BFLD/T1,T2,T3,T4,T5,T6,BZ1,BZ2,BRMAX,CPHI,SPHI,PI2,Y2,MODE,SETB0013
     1VELOC                                                             SETB0014
C  DISTANCES IN CM FOR FIELD PARAMETER ENTRY                             SETB0015
    2 FORMAT(6F12.6)                                                    SETB0016
      PI2=3.1415927/2.0                                                 SETB0017
      READ 2,B 1,BZ2,BRMAX,Y1,PHI,VELOC                                 SETB0018
      PRINT2,BZ1,BZ2,BRMAX,Y1,PHI,VELOC                                 SETB0019
      READ 2,Z1,Z2,Z3,Z4,Z5,Z6                                          SETB0020
      PRINT2,Z1,Z2,Z3,Z4,Z5,Z6                                          SETB0021
      T1=Z1/VELOC                                                       SETB0022
      T2=Z2/VELOC                                                       SETB0023
      T3=Z3/VELOC                                                       SETB0024
      T4=Z4/VELOC                                                       SETB0025
      T5=Z5/VELOC                                                       SETB0026
      T6=Z6/VELOC                                                       SETB0027
C  Y1 IN CM, PHI IN DEGREES                                             SETB0028
      CPHI=COS(PHI*PI2/90.0)                                            SETB0029
      SPHI=SIN(PHI*PI2/90.0)                                            SETB0030
      GO TO(100,200,300),MODE                                           SETB0031
  100 Y2=Y1                                                             SETB0032
      RETURN                                                            SETB0033
  200 Y2=-(Y1/2.0)*PI2*(BZ1-BZ2)/(VELOC*(T2-T1))                        SETB0034
      RETURN                                                            SETB0035
  300 Y2=(BZ1-BZ2)*Y1/(2.0*VELOC*(T2-T1))                               SETB0036
      RETURN                                                            SETB0037
      END                                                               SETB0038


      SUBROUTINE BFIELD(T,BX,BY,BZ)                                     BFLD0010
C  COMPUTES FIELD COMPONENTS AT POSITION Z=VELOC*T, Y=Y1, X=0           BFLD0011
      COMMON/BFLD/T1,T2,T3,T4,T5,T6,BZ1,BZ2,BRMAX,CPHI,SPHI,PI2,Y2,MODE,BFLD0012
     1VELOC                                                             BFLD0013
      COMMON/BFLDP/ZZ(100),BZZ(100),BRR(100),NZ                         BFLD0014
      GO TO(200,300,400),MODE                                           BFLD0015
C  MODE 1    (READ IN TABLES OF BZ,BR)                                  BFLD0016
  200 IF(T.GT.T1) GO TO 100                                             BFLD0017
      BZ=BZ1                                                            BFLD0018
      BY=0.0                                                            BFLD0019
      BX=0.0                                                            BFLD0020
      GO TO 500                                                         BFLD0021
  100 IF(T.GT.T2) GO TO 101                                             BFLD0022
      Z=VELOC*T                                                         BFLD0023
C  TABLE IN GAUSS ON AXIS AND I CM OFF AXIS NORMALIZED TO UNITY BZ(1)   BFLD0024
      CALL TABLE (Z,ZZ(1),NZ,I,MFLAG)                                   BFLD0025
      DBZDZ=(BZZ(I+1)-BZZ(I))/(ZZ(I+1)-ZZ(I))                          BFLD0026
      DBRDZ=(BRR(I+1)-BRR(I))/(ZZ(I+1)-ZZ(I))                          BFLD0027
      BZNORM=BZZ(I)+DBZDZ*(Z-ZZ(I))                                     BFLD0028
      BRNORM=BRR(I)+DBRDZ*(Z-ZZ(I))                                     BFLD0029
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      BZ=BZ2+(BZ1-BZ2)*BZNORM                                          BFLD0030
C  INITIAL RAY DEFINES Y-Z PLANE                                       BFLD0031
      BY=Y2*(BZ1-BZ2)*BRNORM                                           BFLD0032
      BX=0.0                                                           BFLD0033
      GO TO 500                                                        BFLD0034
  101 BZ=BZ2                                                           BFLD0035
      BY=0.0                                                           BFLD0036
      BX=0.0                                                           BFLD0037
      GO TO 500                                                        BFLD0038
C  MODE 2   (COSINE-SQUARED FIELD DECAY)                               BFLD0039
  300 IF(T.GT.T1) GO TO 301                                            BFLD0040
      BX=0.0                                                           BFLD0041
      BY=0.0                                                           BFLD0042
      BZ=BZ1                                                           BFLD0043
      GO TO 500                                                        BFLD0044
  301 IF(T.GT.T2) GO TO 302                                            BFLD0045
      ARG=PI2*(T-T1)/(T2-T1)                                           BFLD0046
      BZ=BZ2+(BZ1-BZ2)*COS(ARG)**2                                     BFLD0047
      BY=Y2*SIN(2.0*ARG)                                               BFLD0048
      BX=0.0                                                           BFLD0049
      GO TO 500                                                        BFLD0050
  302 BX=0.0                                                           BFLD0051
      BY=0.0                                                           BFLD0052
      BZ=BZ2                                                           BFLD0053
      GO TO 500                                                        BFLD0054
C  MODE 3   (EXPONENTIAL FIELD DECAY)                                  BFLD0055
  400 IF(T.GT.T1) GO TO 401                                            BFLD0056
      BX=0.0                                                           BFLD0057
      BY=0.0                                                           BFLD0058
      BZ=BZ1                                                           BFLD0059
      GO TO 500                                                        BFLD0060
  401 EARG=EXP(-(T-T1)/(T2-T1))                                        BFLD0061
      BZ=(BZ1-BZ2)*EARG+BZ2                                            BFLD0062
      BX=0.0                                                           BFLD0063
      BY=Y2*EARG                                                       BFLD0064
C  START TRANSVERSE COMPONENT.  PHI IS ANGLE WITH RESPECT TO X AXIS     BFLD0065
C  INCIDENT BEAM IN Y-Z PLANE                                          BFLD0066
  500 IF(BRMAX.EQ.0.0)RETURN                                           BFLD0067
      IF(T.GT.T3) GO TO 501                                            BFLD0068
      BR=0.0                                                           BFLD0069
      GO TO 505                                                        BFLD0070
  501 IF(T.GT.T4) GO TO 502                                            BFLD0071
      BR=BRMAX*SIN(PI2*(T-T3)/(T4-T3))**2                              BFLD0072
      GO TO 505                                                        BFLD0073
  502 BR=BRMAX                                                         BFLD0074
  505 BY=BR*SPHI+BY                                                    BFLD0075
      BX=BR*CPHI+BX                                                    BFLD0076
      RETURN                                                           BFLD0077
      END                                                              BFLD0078


      SUBROUTINE DERIV(T,V,FD)                                         DERI0010
C  COMPUTES THE FIRST DERIVATIVE OF THE STATE VECTOR FOR USE BY INTEG   DERI0011
      DIMENSION V(30),FD(30)                                           DERI0012
      COMMON/BLOCK1/A1,A2,A3,A4,C1,RO                                  DERI0013
      COMMON/BLOCK3/M,NN                                               DERI0014
      COMPLEX B1,B2,B3,B4,B5,B6,BPLUS,BMINUS,C1,BDOT                   DERI0015
      CALL BFIELD(T,BX,BY,BZ)                                          DERI0016
      BPLUS=CMPLX(BX,BY)                                               DERI0017
      BMINUS=CONJG(BPLUS)                                              DERI0018
      IF(M.EQ.2) GO TO 100                                             DERI0019
C  SPIN 1/2 SECTION                                                    DERI0020
C  A1=0.5*(1+K)     A2=0.5*(1-K)          A3=0.5*K          A4=0.0      DERI0021
C  B0=DELTAW/(MU*GJ)                      C1=MU*GJ/(HBAR*I)  UNITS 1/MICRODERI0022
      B1=CMPLX(V(1),V(2))                                              DERI0023
      B2=CMPLX(V(3),V(4))                                              DERI0024
      B3=CMPLX(V(5),V(6))                                              DERI0025
      B4=CMPLX(V(7),V(8))                                              DERI0026
      BDOT=C1*((A1*BZ+0.25*B0)*B1+A3*BPLUS*B2+0.5*BPLUS*B4)            DERI0027
      FD(1)=REAL(BDOT)                                                 DERI0028
      FD(2)=AIMAG(BDOT)                                                DERI0029
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      BDOT=C1*(A3*BMINUS*B1+(A2*BZ-0.25*B0)*B2+0.5*BPLUS*B3+0.5*B0*B4)   DERI0030
      FD(3)=REAL(BDOT)                                                  DERI0031
      FD(4)=AIMAG(BDOT)                                                 DERI0032
      BDOT=C1*(0.5*BMINUS*B2+(0.25*B0-A1*BZ)*B3+A3*BMINUS*B4)           DERI0033
      FD(5)=REAL(BDOT)                                                  DERI0034
      FD(6)=AIMAG(BDOT)                                                 DERI0035
      BDOT=C1*(0.5*BMINUS*B1+0.5*B0*B2+A3*BPLUS*B3-(A2*BZ+0.25*B0)*B4)  DERI0036
      FD(7)=REAL(BDOT)                                                  DERI0037
      FD(8)=AIMAG(BDOT)                                                 DERI0038
      RETURN                                                            DERI0039
  100 CONTINUE                                                          DERI0040
C   SPIN 1 SECTION                                                      DERI0041
C   A1=0.5*K          A2=0.5-K              A3=K                  A4=SQRT(.5)  DERI0042
C   B0=DELTAW/(1.5*MU*GJ)                   C1=MU*GJ/(HBAR*I)   UNITS 1/MICROSDERI0043
      B1=CMPLX(V(1),V(2))                                               DERI0044
      B2=CMPLX(V(3),V(4))                                               DERI0045
      B3=CMPLX(V(5),V(6))                                               DERI0046
      B4=CMPLX(V(7),V(8))                                               DERI0047
      B5=CMPLX(V(9),V(10))                                              DERI0048
      B6=CMPLX(V(11),V(12))                                             DERI0049
      BDOT=C1*((A1*BZ+0.5*B0)*B1+A3*BPLUS*B2+0.5*BPLUS*B6)              DERI0050
      FD(1)=REAL(BDOT)                                                  DERI0051
      FD(2)=AIMAG(BDOT)                                                 DERI0052
      BDOT=C1*(A3*BMINUS*B1+0.5*BZ*B2+A3*BPLUS*B3+0.5*BPLUS*B5+A4*B0*B4)DERI0053
      FD(3)=REAL(BDOT)                                                  DERI0054
      FD(4)=AIMAG(BDOT)                                                 DERI0055
      BDOT=C1*(A3*BMINUS*B2+(A2*BZ-0.5*B0)*B3+0.5*BPLUS*B4+A4*B0*B5)    DERI0056
      FD(5)=REAL(BDOT)                                                  DERI0057
      FD(6)=AIMAG(BDOT)                                                 DERI0058
      BDOT=C1*(0.5*BMINUS*B3+(0.5*B0-A1*BZ)*B4+A3*BMINUS*B5)            DERI0059
      FD(7)=REAL(BDOT)                                                  DERI0060
      FD(8)=AIMAG(BDOT)                                                 DERI0061
      BDOT=C1*(0.5*BMINUS*B2+A4*B0*B3+A3*BPLUS*B4-0.5*BZ*B5+A3*BMINUS*  DERI0062
     1B6)                                                               DERI0063
      FD(9)=REAL(BDOT)                                                  DERI0064
      FD(10)=AIMAG(BDOT)                                                DERI0065
      BDOT=C1*(0.5*BMINUS*B1+A4*B0*B2+A3*BPLUS*B5-(A2*BZ+0.5*B0)*B6)    DERI0066
      FD(11)=REAL(BDOT)                                                 DERI0067
      FD(12)=AIMAG(BDOT)                                                DERI0068
      RETURN                                                            DERI0069
      END                                                               DERI0070


      SUBROUTINE PRINT(T,VS)                                            PRNT0010
C   PRINTS STRONG FIELD SQUARED AMPLITUDES WITH RESPECT TO PROBLEM DE-  PRNT0011
C   FINED Z AXIS.  STORES WEAK FIELD SQUARED AMPLITUDES WITH RESPECT    PRNT0012
C   TO INSTANTANEOUS B AXIS FOR LATER PRINTOUT BY MAIN PROGRAM          PRNT0013
      COMMON/BLOCK2/BSQ(6,201),TIME(201),BBX(201),BBY(201),BBZ(201),    PRNT0014
     1P2(201),P33(201),PEL(201),N,ITIME                                 PRNT0015
      COMMON/BLOCK3/M,NN                                                PRNT0016
      DIMENSION V(12),VS(12),BBSQ(6)                                    PRNT0017
      ITIME=ITIME+1                                                     PRNT0018
      DO 90 I=1,NN                                                      PRNT0019
   90 V(I)=VS(I)                                                        PRNT0020
      CALL RENORM(N,V,VV)                                               PRNT0021
      IF(VV.GT.1.01) PRINT 80                                           PRNT0022
   80 FORMAT(* RENORMALIZATION EXCEEDS 1 PERCENT*)                      PRNT0023
      CALL BFIELD(T,BX,BY,BZ)                                           PRNT0024
      BBX(ITIME)=BX                                                     PRNT0025
      BBY(ITIME)=BY                                                     PRNT0026
      BBZ(ITIME)=BZ                                                     PRNT0027
      BTOT=SQRT(BX**2+BY**2+BZ**2)                                      PRNT0028
      ALPHA=(3.1415927/180.0)*ARCTAN(BY,BX)                             PRNT0029
      BETA=(3.1415927/180.0)*ARCTAN(SQRT(BX**2+BY**2),BZ)               PRNT0030
      GAMMA=0.0                                                         PRNT0031
      GO TO (101,102,103),M                                             PRNT0032
  101 X=BTOT/63.448                                                     PRNT0033
   98 DPLUS=SQRT(0.5+0.5*X/SQRT(1.0+X**2))                              PRNT0034
      DMINUS=SQRT(0.5-0.5*X/SQRT(1.0+X**2))                             PRNT0035
      DO 105 I=1,4                                                      PRNT0036
  105 BBSQ(I)=V(2*I-1)**2+V(2*I)**2                                     PRNT0037
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      PPEL=BBSQ(1)+BBSQ(2)-BBSQ(3)-BBSQ(4)                                  PRNT0038
      PZ=V(1)**2+V(2)**2+V(7)**2+V(8)**2-V(3)**2-V(4)**2-V(5)**2-V(6)**2PRNT0039
      PZZ=0.0                                                               PRNT0040
      CALL ROT(M,ALPHA,BETA,GAMMA,V)                                        PRNT0041
      QZ=V(1)**2+V(2)**2+V(7)**2+V(8)**2-V(3)**2-V(4)**2-V(5)**2-V(6)**2PRNT0042
      P33(ITIME)=0.0                                                        PRNT0043
      PZ(ITIME)=QZ                                                          PRNT0044
      BSQ(1,ITIME)=V(1)**2+V(2)**2                                          PRNT0045
      BSQ(2,ITIME)=(DPLUS*V(3)+DMINUS*V(7))**2+(DPLUS*V(4)+DMINUS*V(8))*PRNT0046
     1*2                                                                    PRNT0047
      BSQ(3,ITIME)=V(5)**2+V(6)**2                                          PRNT0048
      BSQ(4,ITIME)=(-DMINUS*V(3)+DPLUS*V(7))**2+(-DMINUS*V(4)+DPLUS*V(8)PRNT0049
     1)**2                                                                  PRNT0050
      PEL(ITIME)=BSQ(1,ITIME)+BSQ(2,ITIME)-BSQ(3,ITIME)-BSQ(4,ITIME)        PRNT0051
      GO TO 110                                                             PRNT0052
  102 X=BTOT/14.605                                                         PRNT0053
      DPLUS=(X+1.0/3.0)/SQRT(1.0+2.0*X/3.0+X**2)                            PRNT0054
      DMINUS=(X-1.0/3.0)/SQRT(1.0-2.0*X/3.0+X**2)                           PRNT0055
      E1=SQRT(0.5+0.5*DPLUS)                                                PRNT0056
      E2=SQRT(0.5-0.5*DPLUS)                                                PRNT0057
      E3=SQRT(0.5+0.5*DMINUS)                                               PRNT0058
      E4=SQRT(0.5-0.5*DMINUS)                                               PRNT0059
      DO 104 I=1,6                                                          PRNT0060
  104 BBSQ(I)=V(2*I-1)**2+V(2*I)**2                                         PRNT0061
      PPEL=BBSQ(1)+BBSQ(2)+BBSQ(3)-BBSQ(4)-BBSQ(5)-BBSQ(6)                  PRNT0062
      PZ=V(1)**2+V(2)**2+V(11)**2+V(12)**2-V(5)**2-V(6)**2-V(7)**2-V(8)  PRNT0063
     1*2                                                                    PRNT0064
      PZZ=V(1)**2+V(2)**2+V(5)**2+V(6)**2+V(7)**2+V(8)**2+V(11)**2+V(12)PRNT0065
     1*2-2.0*(V(3)**2+V(4)**2+V(9)**2+V(10)**2)                             PRNT0066
      CALL ROT(M,ALPHA,BETA,GAMMA,V)                                        PRNT0067
      QZ=V(1)**2+V(2)**2+V(11)**2+V(12)**2-V(5)**2-V(6)**2-V(7)**2-V(8)  PRNT0068
     1*2                                                                    PRNT0069
      QZZ=V(1)**2+V(2)**2+V(5)**2+V(6)**2+V(7)**2+V(8)**2+V(11)**2+V(12)PRNT0070
     1*2-2.0*(V(3)**2+V(4)**2+V(9)**2+V(10)**2)                             PRNT0071
      PZ(ITIME)=QZ                                                          PRNT0072
      P33(ITIME)=QZZ                                                        PRNT0073
      BSQ(1,ITIME)=V(1)**2+V(2)**2                                          PRNT0074
      BSQ(2,ITIME)=(E1*V(3)+E2*V(11))**2+(E1*V(4)+E2*V(12))**2              PRNT0075
      BSQ(3,ITIME)=(E3*V(5)+E4*V(9))**2+(E3*V(6)+E4*V(10))**2               PRNT0076
      BSQ(4,ITIME)=V(7)**2+V(8)**2                                          PRNT0077
      BSQ(5,ITIME)=(-E4*V(5)+E3*V(9))**2+(-E4*V(6)+E3*V(10))**2             PRNT0078
      BSQ(6,ITIME)=(-E2*V(3)+E1*V(11))**2+(-E2*V(4)+E1*V(12))**2            PRNT0079
      PEL(ITIME)=BSQ(1,ITIME)+BSQ(2,ITIME)+BSQ(3,ITIME)-BSQ(4,ITIME)        PRNT0080
     1-BSQ(5,ITIME)-BSQ(6,ITIME)                                            PRNT0081
      GO TO 110                                                             PRNT0082
  103 X=BTOT/67.755                                                         PRNT0083
      GO TO 98                                                              PRNT0084
  110 TIME(ITIME)=T                                                         PRNT0085
      PRINT 20,T,BX,BY,BZ,BTOT,PZ,PZZ,PPEL,(BBSQ(I),I=1,N)                 PRNT0086
   20 FORMAT(14F9.4)                                                        PRNT0087
      RETURN                                                                PRNT0088
      END                                                                   PRNT0089


      SUBROUTINE ROT(M,ALPHA,BETA,GAMMA,V)                                  ROT 0010
C  ALPHA, BETA, AND GAMMA ARE EULER ANGLES AS DEFINED BY ROSE, WHICH       ROT 0011
C  ROTATE THE INITIAL COORDINATE SYSTEM INTO THE FINAL SYSTEM.  ALPHA      ROT 0012
C  IS POSITIVE ROTATION ABOUT Z, BETA ABOUT Y PRIME, AND GAMMA ABOUT       ROT 0013
C  Z DOUBLE PRIME                                                          ROT 0014
      DIMENSION V(12),VV(6),WW(6)                                           ROT 0015
      COMPLEX VV,WW,XI,APP,AMM,AMP,APM,CPP,CPO,CPM,COP,COO,COM,CMP,CMO,     ROT 0016
     1CMM                                                                   ROT 0017
      XI=CMPLX(0.0,1.0)                                                     ROT 0018
      APP=COS(0.5*BETA)*CEXP(-XI*0.5*(ALPHA+GAMMA))                         ROT 0019
      AMM=CONJG(APP)                                                        ROT 0020
      AMP=-SIN(0.5*BETA)*CEXP(-XI*0.5*(ALPHA-GAMMA))                        ROT 0021
      APM=-CONJG(AMP)                                                       ROT 0022
      GO TO (10,20,10),M                                                    ROT 0023
   10 DO 11 I=1,4                                                           ROT 0024
   11 VV(I)=CMPLX(V(2*I-1),V(2*I))                                          ROT 0025
      WW(1)=APP*(APP*VV(1)+APM*VV(2))+APM*(APM*VV(3)+APP*VV(4))             ROT 0026
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      WW(2)=APP*(AMP*VV(1)+AMM*VV(2))+APM*(AMM*VV(3)+AMP*VV(4))          ROT 0027
      WW(3)=AMP*(AMP*VV(1)+AMM*VV(2))+AMM*(AMM*VV(3)+AMP*VV(4))          ROT 0028
      WW(4)=AMP*(APP*VV(1)+APM*VV(2))+AMM*(APM*VV(3)+APP*VV(4))          ROT 0029
      DO 12 I=1,4                                                        ROT 0030
      V(2*I-1)=REAL(WW(I))                                               ROT 0031
   12 V(2*I)=AIMAG(WW(I))                                                ROT 0032
      RETURN                                                             ROT 0033
   20 COSB=COS(BETA)                                                     ROT 0034
      SINB=SIN(BETA)                                                     ROT 0035
      CPP=(0.5+0.5*COSB)*CEXP(-XI*(ALPHA+GAMMA))                         ROT 0036
      CP0=(SINB/SQRT(2.0))*CEXP(-XI*GAMMA)                               ROT 0037
      CPM=(0.5-0.5*COSB)*CEXP(XI*(ALPHA-GAMMA))                          ROT 0038
      C0P=(-SINB/SQRT(2.0))*CEXP(-XI*ALPHA)                              ROT 0039
      C00=COSB                                                           ROT 0040
      C0M=-CONJG(C0P)                                                    ROT 0041
      CMP=CONJG(CPM)                                                     ROT 0042
      CM0=-CONJG(CP0)                                                    ROT 0043
      CMM=CONJG(CPP)                                                     ROT 0044
      DO 21 I=1,6                                                        ROT 0045
   21 VV(I)=CMPLX(V(2*I-1),V(2*I))                                       ROT 0046
      WW(1)=APP*(CPP*VV(1)+CP0*VV(2)+CPM*VV(3))+APM*(CPM*VV(4)+CP0*VV(5)ROT 0047
     1+CPP*VV(6))                                                        ROT 0048
      WW(2)=APP*(C0P*VV(1)+C00*VV(2)+C0M*VV(3))+APM*(C0M*VV(4)+C00*VV(5)ROT 0049
     1+C0P*VV(6))                                                        ROT 0050
      WW(3)=APP*(CMP*VV(1)+CM0*VV(2)+CMM*VV(3))+APM*(CMM*VV(4)+CM0*VV(5)ROT 0051
     1+CMP*VV(6))                                                        ROT 0052
      WW(4)=AMP*(CMP*VV(1)+CM0*VV(2)+CMM*VV(3))+AMM*(CMM*VV(4)+CM0*VV(5)ROT 0053
     1+CMP*VV(6))                                                        ROT 0054
      WW(5)=AMP*(C0P*VV(1)+C00*VV(2)+C0M*VV(3))+AMM*(C0M*VV(4)+C00*VV(5)ROT 0055
     1+C0P*VV(6))                                                        ROT 0056
      WW(6)=AMP*(CPP*VV(1)+CP0*VV(2)+CPM*VV(3))+AMM*(CPM*VV(4)+CP0*VV(5)ROT 0057
     1+CPP*VV(6))                                                        ROT 0058
      DO 22 I=1,6                                                        ROT 0059
      V(2*I-1)=REAL(WW(I))                                               ROT 0060
   22 V(2*I)=AIMAG(WW(I))                                                ROT 0061
      RETURN                                                             ROT 0062
      END                                                                ROT 0063


      SUBROUTINE RENORM(N,V,VV)                                          RENM0010
C  RENORMALIZES TO REMOVE ACCUMULATED DEVIATION FROM UNITY TOTAL         RENM0011
C  PROBABILITY                                                          RENM0012
      DIMENSION V(12)                                                    RENM0013
      NN=2*N                                                             RENM0014
      VV2=0.0                                                            RENM0015
      DO 10 I=1,N                                                        RENM0016
   10 VV2=VV2+V(2*I-1)**2+V(2*I)**2                                      RENM0017
      VV=SQRT(VV2)                                                       RENM0018
      DO 11 I=1,NN                                                       RENM0019
   11 V(I)=V(I)/VV                                                       RENM0020
      RETURN                                                             RENM0021
      END                                                                RENM0022


      FUNCTION ARCTAN(Y,X)                                               ACTN0010
C  ARCTANGENT ROUTINE, CORRECT IN ALL QUADRANTS, IN DEGREES              ACTN0011
      IF(X)300,301,302                                                   ACTN0012
  300 IF(Y)303,304,304                                                   ACTN0013
  303 ARCTAN=ATAN(Y/X)-3.1415927                                         ACTN0014
      GO TO 30                                                           ACTN0015
  304 ARCTAN=ATAN(Y/X)+3.1415927                                         ACTN0016
      GO TO 308                                                          ACTN0017
  301 IF(Y)305,306,307                                                   ACTN0018
  305 ARCTAN=-3.1415927/2.0                                              ACTN0019
      GO TO 308                                                          ACTN0020
  306 ARCTAN=0.0                                                         ACTN0021
      GO TO 30                                                           ACTN0022
  307 ARCTAN=3.1415927/2.0                                               ACTN0023
      GO TO 308                                                          ACTN0024
  302 ARCTAN=ATAN(Y/X)                                                   ACTN0025
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  308 ARCTAN=ARCTAN*180.0/3.1415927                                  ACTN0026
      RETURN                                                         ACTN0027
      END                                                            ACTN0028


      SUBROUTINE TABLE (Z,ZZ,NZ,I,MFLAG)                             TBLE0010
C  RETURNS INDEX I OF NEXT SMALLER ENTRY OF ZZ(I)                    TBLE0011
C  MFLAG=0 IF Z=ZZ(I) FOR SOME I                                     TBLE0012
      DIMENSION ZZ(100)                                              TBLE0013
      NJ=10                                                          TBLE0014
      MFLAG=1                                                        TBLE0015
      IF(Z.LT.ZZ(1)) GO TO 30                                        TBLE0016
      IF(Z.GT.ZZ(NZ)) GO TO 30                                       TBLE0017
      DO 10 I=11,NZ,10                                               TBLE0018
      IF(Z.EQ. ZZ(I)) MFLAG=0                                        TBLE0019
      IF(Z.LT.ZZ(I)) GO TO 20                                        TBLE0020
   10 CONTINUE                                                       TBLE0021
      NJ=NZ-I                                                        TBLE0022
      GO TO 11                                                       TBLE0023
   20 I=I-10                                                         TBLE0024
   11 DO 21 J=1,NJ                                                   TBLE0025
      IF(Z.EQ.ZZ(I+J)) MFLAG=0                                       TBLE0026
      IF(Z.LT.ZZ(I+J)) GO TO 40                                      TBLE0027
   21 CONTINUE                                                       TBLE0028
   40 I=I+J-1                                                        TBLE0029
      RETURN                                                         TBLE0030
   30 PRINT 31                                                       TBLE0031
   31 FORMAT(* Z OUT OF RANGE OF TABLE*)                             TBLE0032
      I=1                                                            TBLE0033
      RETURN                                                         TBLE0034
      END                                                            TBLE0035


      SUBROUTINE INTEG(NN,TI,TTF,HH,HHP,MM,VVM,ABS,REL,X0,TT,XYP)    INTE0010
C  INTEG SOLVES A SYSTEM OF NN FIRST ORDER DIFFFRENTIAL EQUATIONS BY  INTE0011
C  A 4TH ORDER ADAMS PREDICTOR-CORRECTOR METHOD WITH AUTOMATIC ERROR  INTE0012
C  CONTROL.  STARTING IS BY THE RUNGA-KUTTA METHOD                   INTE0013
      LOGICAL ACC                                                    INTE0014
      COMMON/INT/N,T,TF,H,H0,HP,M,VM,J,ACC,XLB,RELTST,ABSTST,FACTOR,BND,INTE0015
     1X(30,5),F(30,5),F(30),XP(30),G(30,4),IDOUBL,NDOUBL             INTE0016
      DIMENSION X0(30),XYP(30)                                       INTE0017
C  SET UP INITIAL VALUES                                             INTE0018
      N=NN                                                           INTE0019
      TF=TTF                                                         INTE0020
      H=HH                                                           INTE0021
      HP=HHP                                                         INTE0022
      M=MM                                                           INTE0023
      VM=VVM                                                         INTE0024
      DO 10 I=1,N                                                    INTE0025
   10 X(I,1)=X0(I)                                                   INTE0026
      T=TI                                                           INTE0027
      BND=TI+HP                                                      INTE0028
      H0=H                                                           INTE0029
      ABSTST=ABS                                                     INTE0030
      RELTST=REL                                                     INTE0031
      FACTOR=RELTST/ABSTST                                           INTE0032
      XLB=0.005*RELTST                                               INTE0033
      IDOUBL=0                                                       INTE0034
      NDOUBL=3                                                       INTE0035
      H=2.0*H                                                        INTE0036
   30 CALL START(IRETRN)                                             INTE0037
      GO TO (100,99),IRETRN                                          INTE0038
C  SHOULD ANY OF THE STARTING VALUES BE PRINTED OUT                  INTE0039
  100 T=T-3.0*H                                                      INTE0040
      DO 35 J=2,4                                                    INTE0041
      T=T+H                                                          INTE0042
      CALL TEST(IRETRN)                                              INTE0043
      GO TO (35,60),IRETRN                                           INTE0044
   35 CONTINUE                                                       INTE0045
```

```
C  BEGIN ADAMS METHOD                                                    INTE0046
   40 CALL ADAMS                                                         INTE0047
      CALL ACCRY                                                         INTE0048
      IF (ACC) GO TO 50                                                  INTE0049
      DO 45 I=1,N                                                        INTE0050
   45 X(I,1)=X(I,4)                                                      INTE0051
      GO TO 30                                                           INTE0052
   50 CALL TEST(IRETRN)                                                  INTE0053
      GO TO (101,60),IRETRN                                              INTE0054
  101 CALL DOUBLE(IRETRN)                                                INTE0055
      GO TO (40,30),IRETRN                                               INTE0056
   60 IF (J.EQ.5) GO TO 65                                               INTE0057
      DO 64 I=1,N                                                        INTE0058
   64 XP(I)=X(I,J)                                                       INTE0059
   65 CALL PRINT(T,XP)                                                   INTE0060
      TT=T                                                               INTE0061
      DO 70 I=1,N                                                        INTE0062
   70 XXP(I)=XP(I)                                                       INTE0063
   99 RETURN                                                             INTE0064
      END                                                                INTE0065


      SUBROUTINE START (IRETRN)                                          STRT0010
C  RUNGA-KUTTA STARTING METHOD                                           STRT0011
      LOGICAL ACC                                                        STRT0012
      COMMON/INT/N,T,TF,H,H0,HP,M,VM,J,ACC,XLB,RELTST,ABSTST,FACTOR,BND,STRT0013
     1X(30,5),F(30,5),F(30),XP(30),G(30,4),IDOUBL,NDOUBL                 STRT0014
      J=2                                                                STRT0015
      CALL RNGA                                                          STRT0016
   10 DO 15 I=1,N                                                        STRT0017
   15 XP(I)=X(I,2)                                                       STRT0018
C  XP(I)=DBL INTERVAL RESULT FOR ERROR ANALYSIS                          STRT0019
      T=T-H                                                              STRT0020
      H=0.5*H                                                            STRT0021
      IF ((T+H).NE.T) GO TO 30                                           STRT0022
      PRINT 20                                                           STRT0023
   20 FORMAT(50H EQNS CANNOT BE SOLVED FURTHER WITHIN GIVEN ERROR  )     STRT0024
      TPLUSH=T+H                                                         STRT0025
      PRINT 21,TPLUSH,T                                                  STRT0026
   21 FORMAT(6H T+H=  E15.10,  6H T=    E15.10 )                       STRT0027
      IRETRN=2                                                           STRT0028
      RETURN                                                             STRT0029
   30 DO 40 J=2,3                                                        STRT0030
   40 CALL RNGA                                                          STRT0031
   41 CALL ACCRY                                                         STRT0032
      IF (.NOT.ACC) GO TO 10                                             STRT0033
      J=4                                                                STRT0034
      CALL RNGA                                                          STRT0035
      IRETRN=1                                                           STRT0036
      RETURN                                                             STRT0037
      END                                                                STRT0038


      SUBROUTINE RNGA                                                    RNGA0010
C  INTEGRATE N EQNS AHEAD ON THE J/TH STEP OF LENGTH H.                  RNGA0011
      COMMON/INT/N,T,TF,H,H0,HP,M,VM,J,ACC,XLB,RELTST,ABSTST,FACTOR,BND,RNGA0012
     1X(30,5),F(30,5),F(30),XP(30),G(30,4),IDOUBL,NDOUBL                 RNGA0013
      CALL DERIV(T,X(1,J-1),F(1,J-1))                                    RNGA0014
      DO 10 I=1,N                                                        RNGA0015
      G(I,1)=H*F(I,J-1)                                                  RNGA0016
   10 X(I,J)=X(I,J-1)+0.5*G(I,1)                                         RNGA0017
      TT=T+0.5*H                                                         RNGA0018
      CALL DERIV(TT,X(1,J),F(1,J))                                       RNGA0019
      DO 20 I=1,N                                                        RNGA0020
      G(I,2)=H*F(I,J)                                                    RNGA0021
   20 X(I,J)=X(I,J-1)+0.5*G(I,2)                                         RNGA0022
      CALL DERIV(TT,X(1,J),F(1,J))                                       RNGA0023
      DO 30 I=1,N                                                        RNGA0024
      G(I,3)=H*F(I,J)                                                    RNGA0025
   30 X(I,J)=X(I,J-1)+G(I,3)                                             RNGA0026
```

```
      T=T+H                                                              RNGA0027
      CALL DERIV(T,X(1,J),F(1,1))                                        RNGA0028
      DO 40 I=1,N                                                        RNGA0029
      G(I,4)=H*F(I,J)                                                    RNGA0030
   40 X(I,J)=X(I,J-1)+(G(I,1)+2.0*(G(I,2)+G(I,3))+G(I,4))/6.0            RNGA0031
      RETURN                                                             RNGA0032
      END                                                                RNGA0033


      SUBROUTINE ACCRY                                                   ACCY0010
C  TESTS ABS AND REL ERROR AND SETS ACC .FALSE. IF NEITHER SATISFIED     ACCY0011
      LOGICAL ACC                                                        ACCY0012
      COMMON/INT/N,T,TF,H,H0,HB,M,VM,J,ACC,XLB,RELTST,ABSTST,FACTOR,BND,ACCY0013
     1X(30,5),F(30,5),E(30),XP(30),G(30,4),IDOUBL,NDOUBL                 ACCY0014
      ACC=.TRUE.                                                         ACCY0015
      DO 50 I=1,N                                                        ACCY0016
      E(I)=ABS(XP(I)-X(I,J))                                             ACCY0017
      IF (E(I).GE.ABS(X(I,J))*RELTST) GO TO 10                           ACCY0018
      E(I)=E(I)/ABS(X(I,J))                                              ACCY0019
      GO TO 50                                                           ACCY0020
   10 IF (E(I).GE.ABSTST) GO TO 20                                       ACCY0021
      E(I)=E(I)*FACTOR                                                   ACCY0022
      GO TO 50                                                           ACCY0023
   20 T=T-H                                                              ACCY0024
      H0=0.5*H                                                           ACCY0025
      ACC=.FALSE.                                                        ACCY0026
   75 FORMAT(1H , 16HSTEP SIZE CUT TO, F12.8, 6H AT T=, F12.8)           ACCY0027
C     PRINT 75,H0,T                                                     ACCY0028
      GO TO 99                                                           ACCY0029
   50 CONTINUE                                                           ACCY0030
   99 RETURN                                                             ACCY0031
      END                                                                ACCY0032


      SUBROUTINE TEST (IRETRN)                                           TEST0010
C  MONITORS FOR VM, END OF INTEGN OR PRINT RANGE.                        TEST0011
      COMMON/INT/N,T,TF,H,H0,HB,M,VM,J,ACC,XLB,RELTST,ABSTST,FACTOR,BND,TEST0012
     1X(30,5),F(30,5),F(30),XP(30),G(30,4),IDOUBL,NDOUBL                 TEST0013
      DIMENSION X1(30),X2(30),F1(30),F2(30)                              TEST0014
      IF (M.EQ.0) GO TO 20                                               TEST0015
      IF ((X(M,J).LE.VM).AND.(X(M,J-1).GT.VM)) GO TO 10                  TEST0016
      IF ((X(M,J).GT.VM).AND.(X(M,J-1).LE.VM)) GO TO 10                  TEST0017
      GO TO 20                                                           TEST0018
   10 CALL DIODE                                                         TEST0019
      IF(T-TF)70,70,30                                                   TEST0020
   70 IRETRN=2                                                           TEST0021
      RETURN                                                             TEST0022
   20 IF(ABS((T-TF)/TF)-1.0E-6) 80,81,81                                 TEST0023
   80 IRETRN=2                                                           TEST0024
      RETURN                                                             TEST0025
   81 IF(T.LE.TF) GO TO 40                                               TEST0026
   30 H=TF-T                                                             TEST0027
      DO 35 I=1,N                                                        TEST0028
   35 X(I,1)=X(I,J)                                                      TEST0029
      J=2                                                                TEST0030
      CALL RNGA                                                          TEST0031
      IRETRN=2                                                           TEST0032
      RETURN                                                             TEST0033
   40 IF(T.LT.BND) GO TO 50                                              TEST0034
C  SAVE ALL VARIABLES WHICH MAY BE MODIFIED IN PRINT PROCEDURE           TEST0035
      HSAVE=H                                                            TEST0036
      TSAVE=T                                                            TEST0037
      JSAVE=J                                                            TEST0038
      DO 45 I=1,N                                                        TEST0039
      X1(I)=X(I,1)                                                       TEST0040
      X2(I)=X(I,2)                                                       TEST0041
      F1(I)=F(I,1)                                                       TEST0042
      F2(I)=F(I,2)                                                       TEST0043
   45 X(I,1)=X(I,J)                                                      TEST0044
```

```
      J=2                                                               TEST0045
      H=HND-T                                                           TEST0046
      CALL RNGA                                                         TEST0047
      CALL PRINT(T,X(1,1))                                              TEST0048
      HND=RND+HD                                                        TEST0049
C  RESTORE VARIABLES TO PROCEED                                         TEST0050
      J=JSAVE                                                           TEST0051
      H=HSAVE                                                           TEST0052
      T=TSAVE                                                           TEST0053
      DO 46 I=1,N                                                       TEST0054
      X(I,1)=X1(I)                                                      TEST0055
      X(I,2)=X2(I)                                                      TEST0056
      F(I,1)=F1(I)                                                      TEST0057
   46 F(I,2)=F2(I)                                                      TEST0058
   50 IF (J.NE.5) GO TO 99                                              TEST0059
      DO 60 I=1,N                                                       TEST0060
      X(I,4)=X(I,5)                                                     TEST0061
      DO 60 J=2,5                                                       TEST0062
   60 F(I,J-1)=F(I,J)                                                   TEST0063
   99 IRETRN=1                                                          TEST0064
      RETURN                                                            TEST0065
      END                                                               TEST0066


      SUBROUTINE DIODE                                                  DIOD0010
C  FIND VALUE OF T WHERE THE M/TH VARIABLE REACHES THE VALUE VM         DIOD0011
      COMMON/INT/N,T,TF,H,H0,HD,M,VM,J,ACC,XLB,RELTST,ABSTST,FACTOR,RND,DIOD0012
     1X(30,5),F(30,5),F(30),XP(30),G(30,4),IDOUBL,NDOUBL                DIOD0013
      DIMENSION D(30)                                                   DIOD0014
      Y1=X(M,J)                                                         DIOD0015
      Y0=X(M,J-1)                                                       DIOD0016
      DELT=-ABS(H*Y1/(Y1-Y0))                                           DIOD0017
   10 H=DELT                                                            DIOD0018
      DO 20 I=1,N                                                       DIOD0019
   20 X(I,1)=X(I,J)                                                     DIOD0020
      J=2                                                               DIOD0021
      CALL RNGA                                                         DIOD0022
      CALL DERIV(T,X(1,1),D)                                            DIOD0023
      DELT=(VM-X(M,J))/D(M)                                             DIOD0024
      IF (ABS(DELT).GE.1.0E-4) GO TO 10                                 DIOD0025
      X(M,J)=VM                                                         DIOD0026
      RETURN                                                            DIOD0027
      END                                                               DIOD0028


      SUBROUTINE ADAMS                                                  ADAM0010
C  INTEGRATE ONE STEP BY THE ADAMS PREDICTOR-CORRECTOR METHOD           ADAM0011
      COMMON/INT/N,T,TF,H,H0,HD,M,VM,J,ACC,XLB,RELTST,ABSTST,FACTOR,RND,ADAM0012
     1X(30,5),F(30,5),F(30),XP(30),G(30,4),IDOUBL,NDOUBL                ADAM0013
      J=5                                                               ADAM0014
      CALL DERIV(T,X(1,4),F(1,4))                                       ADAM0015
      DO 10 I=1,N                                                       ADAM0016
   10 XP(I)=X(I,4)+0.041666667*H*(55.0*F(I,4)-59.0*F(I,3)               ADAM0017
     1+37.0*F(I,2)-9.0*F(I,1))                                          ADAM0018
      T=T+H                                                             ADAM0019
      CALL DERIV(T,XP,F(1,5))                                           ADAM0020
      DO 20 I=1,N                                                       ADAM0021
   20 X(I,5)=X(I,4)+0.041666667*H*(9.0*F(I,5)+19.0*F(I,4)               ADAM0022
     1-5.0*F(I,3)+F(I,2))                                               ADAM0023
      RETURN                                                            ADAM0024
      END                                                               ADAM0025


      SUBROUTINE DOUBLE (IRETRN)                                        DBLE0010
C  TEST TO SEE IF INTERVAL CAN BE DOUBLED                               DBLE0011
      COMMON/INT/N,T,TF,H,H0,HD,M,VM,J,ACC,XLB,RELTST,ABSTST,FACTOR,RND,DBLE0012
     1X(30,5),F(30,5),F(30),XP(30),G(30,4),IDOUBL,NDOUBL                DBLE0013
      IDOUBL=IDOUBL+1                                                   DBLE0014
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```
      IF(IDOUBL.LT.NDOUBL) GO TO 99                                    DBLE0015
C  ALLOWS DOUBLE ATTEMPT ONLY EVERY NDOUBL/TH CALL                     DBLE0016
      IDOUBL=0                                                         DBLE0017
      DO 10 I=1,N                                                      DBLE0018
      IF (E(I).GT.XLB)GO TO 99                                         DBLE0019
   10 CONTINUE                                                         DBLE0020
      D1=HP/(2.0*H)                                                    DBLE0021
      IF(D1.LE.2.0) GO TO 99                                           DBLE0022
      D2=(RND-T)/(2.0*H)                                               DBLE0023
      IF(D2.LE.2.0) GO TO 99                                           DBLE0024
      DO 20 I=1,N                                                      DBLE0025
   20 X(I,1)=X(I,4)                                                    DBLE0026
      HO=2.0*H                                                         DBLE0027
      H=2.0*HO                                                         DBLE0028
   30 FORMAT(18H STEP INCREASED TO   F12.8, 6H AT T= F12.8)            DBLE0029
C     PRINT 30,HO,T                                                    DBLE0030
      IRETRN=2                                                         DBLE0031
      RETURN                                                           DBLE0032
   99 IRETRN=1                                                         DBLE0033
      RETURN                                                           DBLE0034
      END                                                              DBLE0035
```