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Majorana Depolarization of
Hydrogen, Deuterium, or Tritium Atoms

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Gerald G. Ohlsen

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MAJORANA DEPOLARIZATION OF HYDROGEN, DEUTERIUM, OR TRITIUM ATOMS

by

Gerald G. Ohlsen

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.

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 (~ 30 cm/ μ sec).

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 Schrodinger equation for a one-electron atom may be written

$$(H_0 + H_1)\psi = i\hbar \frac{\partial \psi}{\partial t}, \quad (1)$$

where H_0 is that part of the Hamiltonian which does not depend on electronic or on nuclear spin and where

$$H_1 = (\mu_0 g_J \vec{J} + \mu_N g_I \vec{I}) \cdot \vec{B} + \alpha(\vec{I} \cdot \vec{J}). \quad (2)$$

In the above expression $\mu_0 = e\hbar/2mc$ (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):

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

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 $H_0 u_n = E_0 u_n$, we may write the general wave function as

$$\Psi = \sum_n b_n u_n e^{-iE_0 t/\hbar} \quad (4)$$

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_0 . 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:

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

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 becomes¹

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

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

$$\begin{aligned} & + \frac{1}{2} \mu_O g_J (B_x - iB_y) [(J-m_J)(J+m_J+1)]^{\frac{1}{2}} b_{m_I, m_J+1} \\ & + \frac{1}{2} \mu_O g_J (B_x + iB_y) [(J+m_J)(J-m_J+1)]^{\frac{1}{2}} b_{m_I, m_J-1} \\ & + \frac{1}{2} \mu_N g_I (B_x - iB_y) [(I-m_I)(I+m_I+1)]^{\frac{1}{2}} b_{m_I+1, m_J} \\ & + \frac{1}{2} \mu_N g_I (B_x + iB_y) [(I+m_I)(I-m_I+1)]^{\frac{1}{2}} b_{m_I-1, m_J} \\ & + \frac{1}{2} \alpha [(I-m_I)(I+m_I+1)(J+m_J)(J-m_J+1)]^{\frac{1}{2}} b_{m_I+1, m_J-1} \\ & + \frac{1}{2} \alpha [(I+m_I)(I-m_I+1)(J-m_J)(J+m_J+1)]^{\frac{1}{2}} b_{m_I-1, m_J+1} \end{aligned}$$

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

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

$$B_0 = \frac{\alpha}{\mu_O g_J}$$

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

TABLE I

HYPERFINE STRUCTURE PARAMETERS

State	g_I	g_J	ϵ	B_I	ΔW	k	B_0
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:

$$\begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \\ b_6 \end{bmatrix} = \frac{\mu_0 g_J}{i\hbar} \begin{bmatrix} (\frac{1}{2}+k)B_z + \frac{1}{2}B_0 & kB_+ & 0 \\ kB_- & \frac{1}{2}B_z & kB_+ \\ 0 & kB_- & (\frac{1}{2}-k)B_z - \frac{1}{2}B_0 \\ 0 & 0 & \frac{1}{2}B_- \\ 0 & \frac{1}{2}B_- & B_0/\sqrt{2} \\ \frac{1}{2}B_- & B_0/\sqrt{2} & 0 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \\ b_6 \end{bmatrix}, \quad (9)$$

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_0 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

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

$$W = -\frac{1}{6}\Delta W \pm \frac{1}{2}\Delta W(1+2m_F x + x^2)^{\frac{1}{2}} + \epsilon \Delta W m_F x, \quad (10)$$

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 $B_1 = \Delta W/[(1-k)\mu_0 g_J] \equiv B_0/(1-k)$ and $\epsilon = k/(1-k)$. For

$$\begin{bmatrix} 0 & 0 & \frac{1}{2}B_+ \\ 0 & \frac{1}{2}B_+ & B_0/\sqrt{2} \\ \frac{1}{2}B_+ & B_0/\sqrt{2} & 0 \\ -(\frac{1}{2}+k)B_z + \frac{1}{2}B_0 & kB_- & 0 \\ kB_+ & -\frac{1}{2}B_z & kB_- \\ 0 & kB_+ & -(\frac{1}{2}-k)B_z - \frac{1}{2}B_0 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \\ b_6 \end{bmatrix}, \quad (9)$$

deuterium atoms we have

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

The definitions of x and of ϵ remain the same, but in this case we have $B_1 = 3B_0/[2(1-k)]$. 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. 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

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

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

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

$$\begin{bmatrix} b'_1 \\ b'_2 \\ b'_3 \\ b'_4 \\ b'_5 \\ b'_6 \end{bmatrix} = \begin{bmatrix} a_{++}c_{++} & a_{++}c_{+0} & a_{++}c_{+-} \\ a_{++}c_{0+} & a_{++}c_{00} & a_{++}c_{0-} \\ a_{++}c_{-+} & a_{++}c_{-0} & a_{++}c_{--} \\ a_{-+}c_{++} & a_{-+}c_{+0} & a_{-+}c_{+-} \\ a_{-+}c_{0+} & a_{-+}c_{00} & a_{-+}c_{0-} \\ a_{-+}c_{-+} & a_{-+}c_{-0} & a_{-+}c_{--} \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \\ b_6 \end{bmatrix}, \quad (14)$$

where α , β , and γ are the positive Euler angles² 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

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

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

$$\begin{bmatrix} b'_+ \\ b'_0 \\ b'_- \end{bmatrix} = \begin{bmatrix} c_{++} & c_{+0} & c_{+-} \\ c_{0+} & c_{00} & c_{0-} \\ c_{-+} & c_{-0} & c_{--} \end{bmatrix} \begin{bmatrix} b_+ \\ b_0 \\ b_- \end{bmatrix} \quad (15)$$

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

$$\begin{aligned} c_{++} &= (\frac{1}{2} + \frac{1}{2}\cos\beta) \exp[-i(\alpha+\gamma)] \\ c_{+0} &= (\sin\beta/\sqrt{2}) \exp[-i\gamma] \\ c_{+-} &= (\frac{1}{2} - \frac{1}{2}\cos\beta) \exp[i(\alpha-\gamma)] \\ c_{0+} &= -(\sin\beta/\sqrt{2}) \exp[-i\alpha] \\ c_{00} &= \cos\beta \\ c_{0-} &= (\sin\beta/\sqrt{2}) \exp[i\alpha] \\ c_{-+} &= (\frac{1}{2} - \frac{1}{2}\cos\beta) \exp[-i(\alpha-\gamma)] \\ c_{-0} &= -(\sin\beta/\sqrt{2}) \exp[i\gamma] \\ c_{--} &= (\frac{1}{2} + \frac{1}{2}\cos\beta) \exp[i(\alpha+\gamma)]. \end{aligned} \quad (16)$$

The complete rotation matrix for a deuterium atom may be written

$$\begin{bmatrix} a_{-+}c_{+-} & a_{-+}c_{+0} & a_{-+}c_{++} \\ a_{-+}c_{0-} & a_{-+}c_{00} & a_{-+}c_{0+} \\ a_{-+}c_{--} & a_{-+}c_{-0} & a_{-+}c_{-+} \\ a_{--}c_{+-} & a_{--}c_{+0} & a_{--}c_{++} \\ a_{--}c_{0-} & a_{--}c_{00} & a_{--}c_{0+} \\ a_{--}c_{--} & a_{--}c_{-0} & a_{--}c_{-+} \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \\ b_6 \end{bmatrix}, \quad (17)$$

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

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

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

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

where

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

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

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

$$\langle \sigma_z \rangle = |b_1|^2 + |b_4|^2 - |b_2|^2 - |b_3|^2$$

$$\langle \sigma_x \rangle = 2\text{Re}(b_1^* b_2 + b_4^* b_3) \quad (20)$$

$$\langle \sigma_y \rangle = 2\text{Im}(b_1^* b_2 + b_4^* b_3)$$

b) Deuterium Atoms

$$\begin{aligned} \langle S_z \rangle &= P_3 = |b_1|^2 + |b_6|^2 - |b_3|^2 - |b_4|^2 \\ 3\langle S_z \rangle^2 - 2 &= P_{33} = |b_1|^2 + |b_6|^2 + |b_3|^2 + |b_4|^2 \\ &\quad - 2|b_2|^2 - 2|b_5|^2 \end{aligned} \quad (21)$$

$$\langle S_x \rangle = \sqrt{2} \text{Re}(b_1^* b_2 + b_2^* b_3 + b_5^* b_4 + b_6^* b_5)$$

$$\langle S_y \rangle = \sqrt{2} \text{Im}(b_1^* b_2 + b_2^* b_3 + b_5^* b_4 + b_6^* b_5)$$

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

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

where the z axis is defined by the (constant) magnetic field direction, $x = B/B_0$, and $\omega = \Delta W/\hbar$. If the initial conditions are $b_1 = \epsilon_1$, $b_2 = \epsilon_2$, $b_3 = \epsilon_3$, and $b_4 = \epsilon_4$, the general solution may be written

$$\begin{aligned} b_1 &= \epsilon_1 \exp[-i(\frac{1}{2}+x)\frac{1}{2}\omega t] \\ b_2 &= \frac{1}{2}\left\{\epsilon_2(1-x/\beta) - \epsilon_4(1/\beta)\right\} \exp[i(\frac{1}{2}+\beta)\frac{1}{2}\omega t] \\ &\quad + \frac{1}{2}\left\{\epsilon_2(1+x/\beta) + \epsilon_4(1/\beta)\right\} \exp[i(\frac{1}{2}-\beta)\frac{1}{2}\omega t] \\ b_3 &= \epsilon_3 \exp[-i(\frac{1}{2}-x)\frac{1}{2}\omega t] \\ b_4 &= \frac{1}{2}\left\{-\epsilon_2(1/\beta) + \epsilon_4(1+x/\beta)\right\} \exp[i(\frac{1}{2}+\beta)\frac{1}{2}\omega t] \\ &\quad + \frac{1}{2}\left\{\epsilon_2(1/\beta) + \epsilon_4(1-x/\beta)\right\} \exp[i(\frac{1}{2}-\beta)\frac{1}{2}\omega t] \end{aligned} \quad (23)$$

where $\beta = \sqrt{1+x^2}$. Only values of $\epsilon_1 - \epsilon_4$ for which $\epsilon_1^2 + \epsilon_2^2 + \epsilon_3^2 + \epsilon_4^2 = 1$ correspond to physical initial states.

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

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

where $x = B/B_0$, $\omega = 2\Delta W/(3\hbar)$, 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:

$$\begin{aligned} b_1 &= \epsilon_1 \exp[-i(1+x)\frac{1}{2}\omega t] \\ b_2 &= \frac{1}{2}\left\{\epsilon_2(1-[x+\frac{1}{2}]/\beta_+) + \epsilon_6(\sqrt{2}/\beta_+)\right\} \exp[i(\frac{1}{2}+\beta_+)\frac{1}{2}\omega t] \\ &\quad + \frac{1}{2}\left\{\epsilon_2(1+[x+\frac{1}{2}]/\beta_+) + \epsilon_6(\sqrt{2}/\beta_+)\right\} \exp[i(\frac{1}{2}-\beta_+)\frac{1}{2}\omega t] \\ b_3 &= \frac{1}{2}\left\{\epsilon_3(1-[x-\frac{1}{2}]/\beta_-) - \epsilon_5(\sqrt{2}/\beta_-)\right\} \exp[i(\frac{1}{2}+\beta_-)\frac{1}{2}\omega t] \\ &\quad + \frac{1}{2}\left\{\epsilon_3(1+[x-\frac{1}{2}]/\beta_-) + \epsilon_5(\sqrt{2}/\beta_-)\right\} \exp[i(\frac{1}{2}-\beta_-)\frac{1}{2}\omega t] \\ b_4 &= \epsilon_4 \exp[-i(1-x)\frac{1}{2}\omega t] \\ b_5 &= \frac{1}{2}\left\{-\epsilon_3(\sqrt{2}/\beta_-) + \epsilon_5(1+[x-\frac{1}{2}]/\beta_-)\right\} \exp[i(\frac{1}{2}+\beta_-)\frac{1}{2}\omega t] \\ &\quad + \frac{1}{2}\left\{\epsilon_3(\sqrt{2}/\beta_-) + \epsilon_5(1-[x-\frac{1}{2}]/\beta_-)\right\} \exp[i(\frac{1}{2}-\beta_-)\frac{1}{2}\omega t] \\ b_6 &= \frac{1}{2}\left\{-\epsilon_2(\sqrt{2}/\beta_+) + \epsilon_6(1+[x+\frac{1}{2}]/\beta_+)\right\} \exp[i(\frac{1}{2}+\beta_+)\frac{1}{2}\omega t] \\ &\quad + \frac{1}{2}\left\{\epsilon_2(\sqrt{2}/\beta_+) + \epsilon_6(1-[x+\frac{1}{2}]/\beta_+)\right\} \exp[i(\frac{1}{2}-\beta_+)\frac{1}{2}\omega t] \end{aligned} \quad (25)$$

where $\beta_{\pm} = \sqrt{x^2 \pm x + 9/4}$. Only those values of $\epsilon_1 - \epsilon_6$ for which $\epsilon_1^2 + \epsilon_2^2 + \epsilon_3^2 + \epsilon_4^2 + \epsilon_5^2 + \epsilon_6^2 = 1$ 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:

- "Adiabatic reduction" of a large (longitudinal) to a small (longitudinal) magnetic field;
- Adiabatic reduction of a large (longitudinal) to a small (transverse) magnetic field;
- The sudden zero field crossing technique of polarization enhancement;
- 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 $\mu_0 g_J / \hbar = 2.8 \text{ MHz/G}$, 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

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

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

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.

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).

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

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

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

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

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

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

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

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

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/ μ sec, 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/ μ sec 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 be 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/ μ sec 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 $B_z = 575 e^{-z/2}$, $B_x = 5$. It is somewhat easier to induce depolarization in this case than in the case where the final field is longitudinal, because $\theta (= \tan^{-1} B_r/B_z)$ 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/ μ sec 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/usec 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 Sona³ 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 $\rightarrow$ 4	1 $\rightarrow$ 4
2 $\rightarrow$ 2	2 $\rightarrow$ 3
3 $\rightarrow$ 1	3 $\rightarrow$ 2
4 $\rightarrow$ 4	4 $\rightarrow$ 1
	5 $\rightarrow$ 6
	6 $\rightarrow$ 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 rotation rate is, again,

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

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/ μ sec 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).

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/ μ sec is assumed.

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

$$\langle \sigma_z \rangle = 1. \quad (33)$$

The time dependence of $\langle \sigma_z \rangle$ for an atom initially in state 4 is obtained from the general solution (Eq. 23) with $\epsilon_1 = \epsilon_2 = \epsilon_3 = 0$ and $\epsilon_4 = 1$:

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

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

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

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

$$\langle \sigma_z \rangle = -1, \quad (36)$$

while for an atom initially in state 2

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

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

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

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 added 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 $\epsilon_1 = \epsilon_2 = 1/\sqrt{2}$ and $\epsilon_3 = \epsilon_4 = 0$; if the electron spin is antiparallel to z, $\langle \sigma_x \rangle = -1$ implies $\epsilon_1 = \epsilon_2 = 0$ and $\epsilon_3 = \epsilon_4 = 1/\sqrt{2}$. For the first of these initial conditions we obtain

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

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

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

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

$$\langle \sigma_x \rangle \xrightarrow{x \rightarrow \infty} \cos \frac{\Delta W}{2\hbar} t; \quad (41)$$

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

$$\langle \sigma_x \rangle \xrightarrow{x \rightarrow 0} \frac{1}{2} (1 + \cos \frac{\Delta W}{\hbar} t); \quad (42)$$

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

(43)

where $\beta_{\pm} = (x^2 \pm x + 9/4)^{1/2}$. 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

$$P_3 = \frac{1}{2} \left(1 + \frac{x^2 - x + 5/4}{x^2 + x + 9/4} \right) \quad (\hbar/\Delta W \ll \tau) \quad (44)$$

$$P_{33} = \frac{1}{2} \left(1 + \frac{x^2 + x - 3/4}{x^2 + x + 9/4} \right)$$

Similarly, for $m_I = 0$ we obtain

$$P_3 = \frac{1}{2} \left[\frac{1}{x^2 + x + 9/4} - \frac{1}{x^2 - x + 9/4} \right] \quad (\hbar/\Delta W \ll \tau) \quad (45)$$

$$P_{33} = - \left[\frac{x^2 + x + 3/4}{x^2 + x + 9/4} + \frac{x^2 - x + 3/4}{x^2 - x + 9/4} \right]$$

and, for $m_I = -1$

$$P_3 = -\frac{1}{2} \left[1 + \frac{x^2 - x + 5/4}{x^2 - x + 9/4} \right] \quad (\hbar/\Delta W \ll \tau) \quad (46)$$

$$P_{33} = \frac{1}{2} \left[1 + \frac{x^2 - x - 3/4}{x^2 - x + 9/4} \right]$$

For $\hbar/\Delta W \gg \tau$ 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	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 dis-

cussed 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.

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REFERENCES

1. L. Motz and M. E. Rose, Phys. Rev. **50**, 348 (1936).
2. M. E. Rose, Elementary Theory of Angular Momentum, John Wiley and Sons, Inc., New York (1957), p. 50.
3. P. G. Sona, Energia Nucl. (Milan) **14**, 295 (1967).
4. T. B. Clegg, G. R. Plattner, and W. Haeberli, Nucl. Instr. & Meth. **62**, 343 (1968).
5. H. Meiner, G. Michel, S. E. Darden, and K. Corrigan, Bull. Am. Phys. Soc., Series II, **13**, 557 (1968).

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

$$\mathcal{H} = H_0 + (\nu_O g_J \vec{J} + \nu_N g_I \vec{I}) \cdot \vec{B} + \alpha (\vec{I} \cdot \vec{J}) ,$$

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 $Z = \text{VELOC} \cdot T$, $X = 0$, 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, RGA, 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/BLCK1/A1, A2, A3, A4, C1, R0	MJRN0012
COMMON/BLCK2/RSQ(6, 201), TIME(201), BRX(201), BRV(201), BBZ(201),	MJRN0013
1P3(201), P33(201), PEL(201), N, ITIME	MJRN0014
COMMON/BLCK3/M, NN	MJRN0015
COMMON/BLCK4/T1, T2, T3, T4, T5, T6, BZ1, BZ2, BRMAX, CPHI, SPHI, PI2, Y2, MODE,	MJRN0016
1VELOC	MJRN0017
COMMON/BLCK5/DP/ZZ(100), BZZ(100), BRR(100), NZ	MJRN0018
DIMENSION XO(30), XXP(30), BPL0T(201)	MJRN0019
COMPLEX C1	MJRN0020
1 FORMAT(10I6)	MJRN0021
2 FORMAT(1H1)	MJRN0022
3 FORMAT(* PROTONS *6F14.8)	MJRN0023
4 FORMAT(* NEUTERONS *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

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9 FORMAT(6F12.4) MJRN0031
10 FORMAT(* STRONG FIELD STATE COEFFICIENTS, INITIAL COORDINATE SYSTEM MJRN0032
1M*) MJRN0033
11 FORMAT(* INTERMEDIATE FIELD STATE COEFFICIENTS, COORDINATE SYSTEM MJRN0034
ROTATED SO NEW Z AXIS POINTS ALONG FIELD DIRECTION *) MJRN0035
12 FORMAT(* P3=SQUARE, P3=PLUS, MAG FIELD PARAMS * 12F7.1) MJRN0036
13 FORMAT(* PARTICLE *12,* STATE *12,* INITIAL STRONG FIELD COEFFS * MJRN0037
12F6.3) MJRN0038
15 FORMAT(* Z(CM) THETA PHI BZ B P3 MJRN0039
1 P3 PFL 1 2 3 4 5 MJRN0040
2 A*) 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),RRR(I) MJRN0045
90 PRINT9,ZZ(I),BZZ(I),RRR(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,HMP MJRN0055
PRINT 9,TI,TTF,HMP MJRN0056
CALL SETUPB MJRN0057
CALL BFIELD(TI,BRX(1),BBY(1),BBZ(1)) MJRN0058
HTOT=SQRT(BRX(1)**2+BBY(1)**2+BBZ(1)**2) MJRN0059
A1PHA=0.0 MJRN0060
BETA=(-(3.1415927/180.0)*ARCTAN(SQRT(BRX(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 XN(I)=0.0 MJRN0064
IF(M-2)101,102,103 MJRN0065
Hn=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 154 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 XN(1)=1.0 MJRN0078
GO TO 104 MJRN0079
151 XN(3)=DPLUS MJRN0080
XN(7)=DMINUS MJRN0081
GO TO 104 MJRN0082
152 XN(5)=1.0 MJRN0083
GO TO 104 MJRN0084
153 XN(3)=-DMINUS MJRN0085
XN(7)=DPLUS MJRN0086
GO TO 104 MJRN0087
154 NSTATE=NSTATE-10 MJRN0088
XN(2*NSTATE-1)=1.0 MJRN0089
GO TO 104 MJRN0090
102 Hn=14.605/1.000233 MJRN0091
Rn=(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=RTOT/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
140  X0(1)=1.0
      GO TO 104
141  X0(3)=SQRT(0.5+0.5*DPLUS)
      X0(11)=SQRT(0.5-0.5*DPLUS)
      GO TO 104
142  X0(5)=SQRT(0.5+0.5*DMINUS)
      X0(9)=SQRT(0.5-0.5*DMINUS)
      GO TO 104
143  X0(7)=1.0
      GO TO 104
144  X0(5)=-SQRT(0.5-0.5*DMINUS)
      X0(9)=SQRT(0.5+0.5*DMINUS)
      GO TO 104
145  X0(3)=-SQRT(0.5-0.5*DPLUS)
      X0(11)=SQRT(0.5+0.5*DPLUS)
      GO TO 104
146  NSTATE=NSTATE-10
      X0(2*NSTATE-1)=1.0
      GO TO 104
103  R0=67.755/1.001623
      A1=0.5*(1.0+0.001623/1.001623)
      A2=0.5*(1.0-0.001623/1.001623)
      A3=0.5*0.001623/1.001623
      A4=0.0
      N=4
      PRINT 5,A1,A2,A3,A4,R0
      X=BTOT/67.755
      GO TO 98
104  ARG=2.0*3.1415927*1.401*2.00229
      C1=CMPLX(0.0,-ARG)
C  REFER INITIAL VECTOR TO PROBLEM DEFINED Z AXIS VIA APPROPRIATE ROTATION
      CALL ROT(M,ALPHA,BETA,GAMMA,X0)
      NN=2*N
      PRINT 10
      PRINT 7
      CALL PRINT(TI,X0)
      HH=0.0001
      MM=0
      VVM=0.0
      ABS=1.0E-05
      REL=1.0E-05
      CALL INTER(NN,TI,TTF,HH,HHP,MM,VVM,ABS,REL,X0,TT,XXP)
C  NN  NUMBER OF FIRST ORDER DIFFERENTIAL EQUATIONS
C  TI  INITIAL VALUE OF INDEPENDENT VARIABLE
C  TTF FINAL VALUE OF INDEPENDENT VARIABLE
C  HH  GUESS AT STEP SIZE
C  HHP PRINT STEP SIZE
C  MM  INDEX OF VARIABLE TO BE MONITORED (0 IF NO MONITORING)
C  VVM VALUE TO MONITOR FOR
C  ABS MAXIMUM ACCEPTABLE ABSOLUTE ERROR IN ONE INTEGRATION STEP
C  REL MAXIMUM ACCEPTABLE RELATIVE ERROR IN ONE INTEGRATION STEP
C  X0  VECTOR OF STARTING VALUES
C  TT  VALUE OF INDEPENDENT VARIABLE RETURNED AT END OF INTEGRATION
C  XXP VALUES OF DEPENDENT VARIABLES RETURNED AT END OF INTEGRATION
      PRINT 11
      PRINT 15
      NTIME=TIME
      DO 110 I=1,NTIME
      BTOT=SQRT(BBX(I)**2+BBY(I)**2+BBZ(I)**2)
      POSN=TIME(I)*VELOC
      PHIF=ARCTAN(BBY(I),BBX(I))
      THETAF=ARCTAN(SQRT(BBY(I)**2+BBX(I)**2),BBZ(I))
      PRINT 8,POSN,THETAF,PHIF,BBZ(I),BTOT,P3(I),P33(I),PEL(I),(BSO(J,I)
1, J=1,N)
110 CONTINUE
C  THE FOLLOWING 18 CARDS PRODUCE A PLOT WITH LASL SUBROUTINES
      CALL ADV(1)
      CALL DGA(50,950,50,800,TI,TTF,1.0,0.0)
      CALL DLNLY(10,10)
      CALL SLLIN(10,01)
      CALL SRLIN(10,02)

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DO 120 J=1,N	MJRN0175
DO 121 I=1,NTIME	MJRN0176
121 HPL0T(I)=RSQ(J,I)	MJRN0177
120 CALL PLOT(NTIME,TIME(I),I,BPLOT(I),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(I),I,P33(I),1,16,0)	MJRN0181
CALL PLOT(NTIME,TIME(I),I,P3(I),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,YI,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 SETUPR	SETB0010
C READS IN FIELD PARAMETERS AND COMPUTES SOME FREQUENTLY USED QUAN-	SETB0011
C TITIES FOR USE BY SUBROUTINE BFIELD	SETB0012
COMMON/BFIELD/T1,T2,T3,T4,T5,T6,BZ1,BZ2,BRMAX,CPHI,SPHI,PI2,Y2,MODE	SETB0013
1VFLOC	SETB0014
C DISTANCES IN CM FOR FIELD PARAMETER ENTRY	SETB0015
2 FORMAT(6F12.6)	SETB0016
PI2=3.1415927/2.0	SETB0017
READ 2,B1,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/BFIELD/T1,T2,T3,T4,T5,T6,BZ1,BZ2,BRMAX,CPHI,SPHI,PI2,Y2,MODE	BFLD0012
1VFLOC	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
B7=BZ1	BFLD0018
BX=0.0	BFLD0019
BY=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 1 CM OFF AXIS NORMALIZED TO UNITY BZ(1)	BFLD0024
CALL TABLE(Z,ZZ(1),NZ,1,MFLAG)	BFLD0025
DBZDZ=(BZ7(I+1)-BZZ(I))/(ZZ(I+1)-ZZ(I))	BFLD0026
DBRDZ=(BR7(I+1)-BRR(I))/(ZZ(I+1)-ZZ(I))	BFLD0027
B7NORM=BZ7(I)+DBZDZ*(Z-Z7(I))	BFLD0028
B7NORM=BRR(I)+DBRDZ*(Z-Z7(I))	BFLD0029

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      H7=BZ2*(BZ1-BZ2)*BZNORM
C  INITIAL RAY DEFINES Y-Z PLANE
      BY=Y2*(BZ1-BZ2)*BRNORM
      BX=0.0
      GO TO 500
101 H7=BZ2
      BV=0.0
      BV=0.0
      GO TO 500
C  MODE 2 (COSINE-SQUARED FIELD DECAY)
300 IF (T.GT.T1) GO TO 301
      BX=0.0
      BY=0.0
      H7=BZ1
      GO TO 500
301 IF (T.GT.T2) GO TO 302
      ARG=PI2*(T-T1)/(T2-T1)
      H7=BZ2*(BZ1-BZ2)*COS(ARG)**2
      BY=Y2*SIN(2.0*ARG)
      BV=0.0
      GO TO 500
302 BX=0.0
      BY=0.0
      H7=BZ2
      GO TO 500
C  MODE 3 (EXPONENTIAL FIELD DECAY)
400 IF (T.GT.T1) GO TO 401
      BX=0.0
      BY=0.0
      H7=BZ1
      GO TO 500
401 EARG=EXP(-(T-T1)/(T2-T1))
      H7=(BZ1-BZ2)*EARG*BZ2
      BV=0.0
      BY=Y2*EARG
C  START TRANSVERSE COMPONENT. PHI IS ANGLE WITH RESPECT TO X AXIS
C  INCIDENT BEAM IN Y-Z PLANE
500 IF (BRMAX.EQ.0.0) RETURN
      IF (T.GT.T3) GO TO 501
      BV=0.0
      GO TO 505
501 IF (T.GT.T4) GO TO 502
      BV=BRMAX*SIN(PI2*(T-T3)/(T4-T3))**2
      GO TO 505
502 BV=BRMAX
505 BV=BV*SPHT*BY
      BX=BV*CPHT*BX
      RETURN
      END

```

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      SUBROUTINE DERIV(T,V,FD)
C  COMPUTES THE FIRST DERIVATIVE OF THE STATE VECTOR FOR USE BY INTEG
      DIMENSION V(30),FD(30)
      COMMON/BLACK1/A1,A2,A3,A4,C1,R0
      COMMON/BLACK3/M,NN
      COMPLEX B1,B2,B3,B4,B5,B6,BPLUS,BMINUS,C1,BDOT
      CALL BFIELD(T,BX,BY,BZ)
      BPLUS=CMPLX(BX,BY)
      BMINUS=CONJG(BPLUS)
      IF (M.EQ.2) GO TO 100
C  SPIN 1/2 SECTION
C  A1=0.5*(1+K)      A2=0.5*(1-K)      A3=0.5*K      A4=0.0
C  B0=DELTAW/(MH*GJ)      C1=MH*GJ/(HBAR*T)  UNITS 1/MICROSECONDS
      B1=CMPLX(V(1),V(2))
      B2=CMPLX(V(3),V(4))
      B3=CMPLX(V(5),V(6))
      B4=CMPLX(V(7),V(8))
      BDOT=C1*((A1*BZ+0.25*B0)*B1+A3*BPLUS*B2+0.5*BPLUS*B4)
      FD(1)=REAL(BDOT)
      FD(2)=AIMAG(BDOT)

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      HDOT=C1*(A3*BMINUS*B1+(A2*BZ-0.25*B0)*B2+0.5*BPLUS*B3+0.5*B0*B4)
      FN(3)=REAL(HDOT)
      FN(4)=AIMAG(HDOT)
      HDOT=C1*(0.5*BMINUS*B2+(0.25*B0-A1*BZ)*B3+A3*BMINUS*B4)
      FN(5)=REAL(HDOT)
      FN(6)=AIMAG(HDOT)
      HDOT=C1*(0.5*BMINUS*B1+0.5*B0*B2+A3*BPLUS*B3-(A2*BZ+0.25*B0)*B4)
      FN(7)=REAL(HDOT)
      FN(8)=AIMAG(HDOT)
      RETURN
100 CONTINUE
C SPIN 1 SECTION
C A1=0.5*K      A2=0.5-K      A3=K      A4=SQRT(.5)
C B0=DELTA W/(1.5*MU*GJ)      C1=MU*GJ/(HBAR*T)  UNITS 1/MICROSECOND
      H1=CMPLX(V(1),V(2))
      H2=CMPLX(V(3),V(4))
      H3=CMPLX(V(5),V(6))
      H4=CMPLX(V(7),V(8))
      H5=CMPLX(V(9),V(10))
      H6=CMPLX(V(11),V(12))
      HDOT=C1*(A1*H7+0.5*B0)*B1+A3*BPLUS*B2+0.5*BPLUS*B6)
      FN(1)=REAL(HDOT)
      FN(2)=AIMAG(HDOT)
      HDOT=C1*(A3*BMINUS*B1+0.5*BZ*B2+A3*BPLUS*B3+0.5*BPLUS*B5+A4*B0*B4)
      FN(3)=REAL(HDOT)
      FN(4)=AIMAG(HDOT)
      HDOT=C1*(A3*BMINUS*B2+(A2*BZ-0.5*B0)*B3+0.5*BPLUS*B4+A4*B0*B5)
      FN(5)=REAL(HDOT)
      FN(6)=AIMAG(HDOT)
      HDOT=C1*(0.5*BMINUS*B3+(0.5*B0-A1*BZ)*B4+A3*BMINUS*B5)
      FN(7)=REAL(HDOT)
      FN(8)=AIMAG(HDOT)
      HDOT=C1*(0.5*BMINUS*B2+A4*B0*B3+A3*BPLUS*B4-0.5*BZ*B5+A3*BMINUS*
      B6)
      FN(9)=REAL(HDOT)
      FN(10)=AIMAG(HDOT)
      HDOT=C1*(0.5*BMINUS*B1+A4*B0*B2+A3*BPLUS*B5-(A2*BZ+0.5*B0)*B6)
      FN(11)=REAL(HDOT)
      FN(12)=AIMAG(HDOT)
      RETURN
END

```

```

      SUBROUTINE PRINT(T,VS)
C PRINTS STRONG FIELD SQUARED AMPLITUDES WITH RESPECT TO PROBLEM DE-
C FINED Z AXIS. STORES WEAK FIELD SQUARED AMPLITUDES WITH RESPECT
C TO INSTANTANEOUS R AXIS FOR LATER PRINTOUT BY MAIN PROGRAM
      COMMON/BLOCK5/RSQ(6,201),TIME(201),BRX(201),BRY(201),BBZ(201),
      IP1(201),P33(201),PEL(201),N*ITIME
      COMMON/BLOCK3/M,NN
      DIMENSION V(12),VS(12),BRSQ(6)
      ITIME=ITIME+1
      DO 90 I=1,NN
90  V(I)=VS(I)
      CALL RENORM(N,V,VV)
      IF(VV.GT.1.01) PRINT 80
80  FORMAT(* RENORMALIZATION EXCEEDS 1 PERCENT*)
      CALL BFIELD(T,BX,RY,RZ)
      BRX(ITIME)=RX
      BRY(ITIME)=RY
      BRZ(ITIME)=RZ
      BTOT=SQRT(BX**2+RY**2+RZ**2)
      A1 PHA=(3.1415927/180.0)*ARCTAN(BY,RX)
      BETA=(3.1415927/180.0)*ARCTAN(SQRT(BX**2+RY**2),RZ)
      GAMMA=0.0
      GO TO (101,102,103),M
101 X=BTOT/63.448
      98 BPLUS=SQRT(0.5+0.5*X/SQRT(1.0+X**2))
      BMINUS=SQRT(0.5-0.5*X/SQRT(1.0+X**2))
      DO 105 I=1,4
105  BRSQ(I)=V(2*I-1)**2+V(2*I)**2

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PPEL=BBSQ(1)+BBSQ(2)-BBSQ(3)-BBSQ(4) PRNT0038
P7=V(1)**2+V(2)**2+V(7)**2+V(8)**2-V(3)**2-V(4)**2-V(5)**2-V(6)**2 PRNT0039
PZZ=0.0 PRNT0040
CALL ROT(M,ALPHA,BETA,GAMMA,V) PRNT0041
Q7=V(1)**2+V(2)**2+V(7)**2+V(8)**2-V(3)**2-V(4)**2-V(5)**2-V(6)**2 PRNT0042
P33(ETIME)=0.0 PRNT0043
P3(ETIME)=QZ PRNT0044
BSQ(1,ETIME)=V(1)**2+V(2)**2 PRNT0045
BSQ(2,ETIME)=(DPLUS*V(3)+DMINUS*V(7))**2+(DPLUS*V(4)+DMINUS*V(8))**2 PRNT0046
1*2 PRNT0047
BSQ(3,ETIME)=V(5)**2+V(6)**2 PRNT0048
BSQ(4,ETIME)=(-DMINUS*V(3)+DPLUS*V(7))**2+(-DMINUS*V(4)+DPLUS*V(8))**2 PRNT0049
1)*2 PRNT0050
PFL(ETIME)=BSQ(1,ETIME)+BSQ(2,ETIME)-BSQ(3,ETIME)-BSQ(4,ETIME) 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
P7=V(1)**2+V(2)**2+V(11)**2+V(12)**2-V(5)**2-V(6)**2-V(7)**2-V(8)**2 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)**2 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
Q7=V(1)**2+V(2)**2+V(11)**2+V(12)**2-V(5)**2-V(6)**2-V(7)**2-V(8)**2 PRNT0068
1*2 PRNT0069
Q7Z=V(1)**2+V(2)**2+V(5)**2+V(6)**2+V(7)**2+V(8)**2+V(11)**2+V(12)**2 PRNT0070
1*2-2.0*(V(3)**2+V(4)**2+V(9)**2+V(10)**2) PRNT0071
P3(ETIME)=QZ PRNT0072
P33(ETIME)=QZZ PRNT0073
BSQ(1,ETIME)=V(1)**2+V(2)**2 PRNT0074
BSQ(2,ETIME)=(E1*V(3)+E2*V(11))**2+(E1*V(4)+E2*V(12))**2 PRNT0075
BSQ(3,ETIME)=(E3*V(5)+E4*V(9))**2+(E3*V(6)+E4*V(10))**2 PRNT0076
BSQ(4,ETIME)=V(7)**2+V(8)**2 PRNT0077
BSQ(5,ETIME)=(-E4*V(5)+E3*V(9))**2+(-E4*V(6)+E3*V(10))**2 PRNT0078
BSQ(6,ETIME)=(-E2*V(3)+E1*V(11))**2+(-E2*V(4)+E1*V(12))**2 PRNT0079
PFL(ETIME)=BSQ(1,ETIME)+BSQ(2,ETIME)+BSQ(3,ETIME)+BSQ(4,ETIME) PRNT0080
1-BSQ(5,ETIME)-BSQ(6,ETIME) PRNT0081
GO TO 110 PRNT0082
103 X=BTOT/67.755 PRNT0083
GO TO 98 PRNT0084
110 TIME(ETIME)=T PRNT0085
PRINT 20,T,RX,RY,RZ,BTOT,PZ,PZZ,PPEL,(BBSQ(I),I=1,N) PRNT0086
20 FORMAT(14F9.4) PRNT0087
RETURN PRNT0088
END PRNT0089

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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,CPM,CPO,CPM,COP,CQO,COM,CMP,CMO ROT 0016
1CMM ROT 0017
XI=CMPLX(0.0,1.0) ROT 0018
APP=COS(0.5*PI*ETA)*CEXP(-XI*0.5*(ALPHA+GAMMA)) ROT 0019
AMM=CONJG(APP) ROT 0020
AMP=-SIN(0.5*PI*ETA)*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 COSH=COS(ETA)	ROT 0034
SINB=SIN(ETA)	ROT 0035
CPP=(0.5+0.5*COSH)*CEXP(-XI*(ALPHA+GAMMA))	ROT 0036
CPD=(SINH/SQRT(2.0))*CEXP(-XI*GAMMA)	ROT 0037
CPM=(0.5-0.5*COSH)*CEXP(XI*(ALPHA-GAMMA))	ROT 0038
CPN=(-SINH/SQRT(2.0))*CEXP(-XI*ALPHA)	ROT 0039
CND=COSH	ROT 0040
COM=-CONJG(CPD)	ROT 0041
CMP=CONJG(CPM)	ROT 0042
CND=-CONJG(CPD)	ROT 0043
CMM=CONJG(CPP)	ROT 0044
DO 21 I=1,6	ROT 0045
21 VV(I)=CMP*X(V(2*I-1),V(2*I))	ROT 0046
WW(1)=APP*(CPP*VV(1)+CPD*VV(2)+CPM*VV(3))+APM*(CPM*VV(4)+CPD*VV(5)+CPP*VV(6))	ROT 0047
1+CPP*VV(6))	ROT 0048
WW(2)=APP*(CNP*VV(1)+CND*VV(2)+COM*VV(3))+APM*(COM*VV(4)+CND*VV(5)+CNP*VV(6))	ROT 0049
1+CNP*VV(6))	ROT 0050
WW(3)=APP*(CMP*VV(1)+CND*VV(2)+CMM*VV(3))+APM*(CMM*VV(4)+CND*VV(5)+CMP*VV(6))	ROT 0051
1+CM*VV(6))	ROT 0052
WW(4)=AMP*(CMP*VV(1)+CND*VV(2)+CMM*VV(3))+AMM*(CMM*VV(4)+CND*VV(5)+CMP*VV(6))	ROT 0053
1+CM*VV(6))	ROT 0054
WW(5)=AMP*(CNP*VV(1)+CND*VV(2)+COM*VV(3))+AMM*(COM*VV(4)+CND*VV(5)+CNP*VV(6))	ROT 0055
1+CNP*VV(6))	ROT 0056
WW(6)=AMP*(CPP*VV(1)+CPD*VV(2)+CPM*VV(3))+AMM*(CPM*VV(4)+CPD*VV(5)+CPP*VV(6))	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)	REN0010
C RENORMALIZES TO REMOVE ACCUMULATED DEVIATION FROM UNITY TOTAL	REN0011
C PROBABILITY	REN0012
DIMENSION V(12)	REN0013
NN=2*N	REN0014
VV2=0.0	REN0015
DO 10 I=1,N	REN0016
10 VV2=VV2+V(2*I-1)**2+V(2*I)**2	REN0017
VV=SQRT(VV2)	REN0018
DO 11 I=1,NN	REN0019
11 V(I)=V(I)/VV	REN0020
RETURN	REN0021
END	REN0022

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 305	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 308	ACTN0022
307 ARCTAN=3.1415927/2.0	ACTN0023
GO TO 308	ACTN0024
302 ARCTAN=ATAN(Y/X)	ACTN0025

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308 ADCTAN=ARCTAN*180.0/3.1415927
RETURN
END

```

ACTN0026
ACTN0027
ACTN0028

```

SUBROUTINE TABLE (Z,ZZ,NZ,I,MFLAG)
C RETURNS INDEX I OF NEXT SMALLER ENTRY OF ZZ(I)
C MFLAG=0 IF Z=ZZ(I) FOR SOME I
  DIMENSION ZZ(100)
  NJ=10
  MFLAG=1
  IF(Z.LT.Z7(1)) GO TO 30
  IF(Z.GT.Z7(NZ)) GO TO 30
  DO 10 I=1,NZ,10
  IF(Z.EQ.Z7(I)) MFLAG=0
  IF(Z.LT.Z7(I)) GO TO 20
10 CONTINUE
  NJ=NZ-I
  GO TO 11
20 I=I-10
11 DO 21 J=1,NJ
  IF(Z.EQ.Z7(I+J)) MFLAG=0
  IF(Z.LT.Z7(I+J)) GO TO 40
21 CONTINUE
40 I=I+J-1
  RETURN
30 PRINT 31
31 FORMAT(* 7 OUT OF RANGE OF TABLE*)
  I=1
  RETURN
END

```

TBLE0010
TBLE0011
TBLE0012
TBLE0013
TBLE0014
TBLE0015
TBLE0016
TBLE0017
TBLE0018
TBLE0019
TBLE0020
TBLE0021
TBLE0022
TBLE0023
TBLE0024
TBLE0025
TBLE0026
TBLE0027
TBLE0028
TBLE0029
TBLE0030
TBLE0031
TBLE0032
TBLE0033
TBLE0034
TBLE0035

```

SUBROUTINE INTEG(NN,TI,TTF,HH,HHP,MM,VVM,ABS,REL,X0,TT,XP)
C INTEG SOLVES A SYSTEM OF NN FIRST ORDER DIFFERENTIAL EQUATIONS BY
C A 4TH ORDER ADAMS PREDICTOR-CORRECTOR METHOD WITH AUTOMATIC ERROR
C CONTROL. STARTING IS BY THE RUNGE-KUTTA METHOD
  LOGICAL ACC
  COMMON/INT/N,T,TF,H,H0,HP,M,VM,J,ACC,XLB,RELTST,ABSTST,FACTOR,BND,
  1X(30,5),F(30,5),E(30),XP(30),G(30,4),IDOUBL,NDOURL
  DIMENSION X0(30),XP(30)
C SET UP INITIAL VALUES
  N=NN
  TF=TTF
  H=HH
  HP=HHP
  M=MM
  VM=VVM
  DO 10 I=1,N
10 X(I,1)=X0(I)
  T=TI
  BND=TI+HP
  H0=H
  ABSTST=ABS
  RELTST=REL
  FACTOR=RELTST/ABSTST
  XLB=0.005*RELTST
  IDOUBL=0
  NDOURL=3
  H=2.0*H
30 CALL START(I,RETRN)
  GO TO (100,99),IRETRN
C SHOULD ANY OF THE STARTING VALUES BE PRINTED OUT
100 T=T-3.0*H
  DO 35 J=2,4
  T=T+H
  CALL TEST(I,RETRN)
  GO TO (35,60),IRETRN
35 CONTINUE

```

INTE0010
INTE0011
INTE0012
INTE0013
INTE0014
INTE0015
INTE0016
INTE0017
INTE0018
INTE0019
INTE0020
INTE0021
INTE0022
INTE0023
INTE0024
INTE0025
INTE0026
INTE0027
INTE0028
INTE0029
INTE0030
INTE0031
INTE0032
INTE0033
INTE0034
INTE0035
INTE0036
INTE0037
INTE0038
INTE0039
INTE0040
INTE0041
INTE0042
INTE0043
INTE0044
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(I,RETRN)	INTE0053
GO TO (10,60),IRETRN	INTE0054
101 CALL DOUBLE(I,RETRN)	INTE0055
GO TO (40,30),IRETRN	INTE0056
60 IF (J.EQ.5) GO TO 45	INTE0057
DO 64 I=1,N	INTE0058
64 X(I)=X(I,J)	INTE0059
65 CALL PRINT(T,XP)	INTE0060
TT=T	INTE0061
DO 70 I=1,N	INTE0062
70 XP(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
IX(30,5),F(30,5),F(30),XP(30),G(30,4),IDOUHL,NDOURL	STRT0014
J=2	STRT0015
CALL RUNGA	STRT0016
10 DO 15 I=1,N	STRT0017
15 XP(I)=X(I,2)	STRT0018
C XP(I)=DHL INTERVAL RESULT FOR ERROR ANALYSIS	STRT0019
TT=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 RUNGA	STRT0031
41 CALL ACCRY	STRT0032
IF (.NOT.ACC) GO TO 10	STRT0033
J=4	STRT0034
CALL RUNGA	STRT0035
IRETRN=1	STRT0036
RETURN	STRT0037
END	STRT0038

SUBROUTINE RUNGA	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
IX(30,5),F(30,5),F(30),XP(30),G(30,4),IDOUHL,NDOURL	RNGA0013
CALL DERIV(T,X(I,J-1),F(I,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(I,J),F(I,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(I,J),F(I,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,J))	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,H1,M,VM,J,ACC,XLB,RELTST,ABSTST,FACTOR,BND,	ACCY0013
IX(30,5),F(30,5),E(30),XP(30),G(30,4),IDOUHL,NDOURL	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
H1=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 INTEG. OR PRINT RANGE.	TEST0011
COMMON/INT/N,T,TF,H,H0,H1,M,VM,J,ACC,XLB,RELTST,ABSTST,FACTOR,BND,	TEST0012
IX(30,5),F(30,5),F(30),XP(30),G(30,4),IDOUHL,NDOURL	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) A0,A1,81	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=BND-T	TEST0046
CALL RNGA	TEST0047
CALL PRINT(T,X(1,J))	TEST0048
HND=BND+H	TEST0049
C RESTORE VARIABLES TO PROCEED	TEST0050
J=JSAVE	TEST0051
H=HSAVF	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 (I.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 IOTRN=1	TEST0064
RETURN	TEST0065
END	TEST0066

SUBROUTINE DIODE	DIOD0010
C FIND VALUE OF T WHERE THE MATH VARIABLE REACHES THE VALUE VM	DIOD0011
COMMON/INT/N,T,TF,H,H0,H0,M,VM,J,ACC,XLB,RELTST,ABSTST,FACTOR,BND,DIOD0012	
IX(30,5),F(30,5),F(30),XP(30),G(30,4),IDOURL,NDOURL	DIOD0013
DIMENSION D(30)	DIOD0014
YI=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,J),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,H0,M,VM,J,ACC,XLB,RELTST,ABSTST,FACTOR,BND,ADAM0012	
IX(30,5),F(30,5),F(30),XP(30),G(30,4),IDOURL,NDOURL	ADAM0013
J=5	ADAM0014
CALL DERIV(T,X(1,4),F(1,4))	ADAM0015
DO 10 I=1,N	ADAM0016
10 X(I)=X(I,4)+0.041666667*H*(55.0*F(I,4)-59.0*F(I,3)	ADAM0017
+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
+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,H0,M,VM,J,ACC,XLB,RELTST,ABSTST,FACTOR,BND,DBLE0012	
IX(30,5),F(30,5),F(30),XP(30),G(30,4),IDOURL,NDOURL	DBLE0013
IDOURL=IDOURL+1	DBLE0014

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      IF (IDOURL.LT.NDOURL) GO TO 99
C   ALLOWS DOUBLE ATTEMPT ONLY EVERY NDOURL/TH CALL
      IDOURL=0
      DO 10 I=1,N
      IF (E(I).GT.XL8) GO TO 99
10   CONTINUE
      D1=HP/(2.0*H)
      IF (D1.LE.2.0) GO TO 99
      D2=(RND-T1)/(2.0*H)
      IF (D2.LE.2.0) GO TO 99
      DO 20 I=1,N
20   X(I,1)=X(I,4)
      H0=2.0*H
      H=2.0*H0
30   FORMAT(18H STEP INCREASED TO      F12.8, 6H AT T= F12.8)
C   PRINT 30,H0,T
      IDPTRN=2
      RETURN
99   IDPTRN=1
      RETURN
      END

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DBLE0015
DBLE0016
DBLE0017
DBLE0018
DBLE0019
DBLE0020
DBLE0021
DBLE0022
DBLE0023
DBLE0024
DBLE0025
DBLE0026
DBLE0027
DBLE0028
DBLE0029
DBLE0030
DBLE0031
DBLE0032
DBLE0033
DBLE0034
DBLE0035

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