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**Majorana Depolarization of
Hydrogen, Deuterium, or Tritium Atoms**

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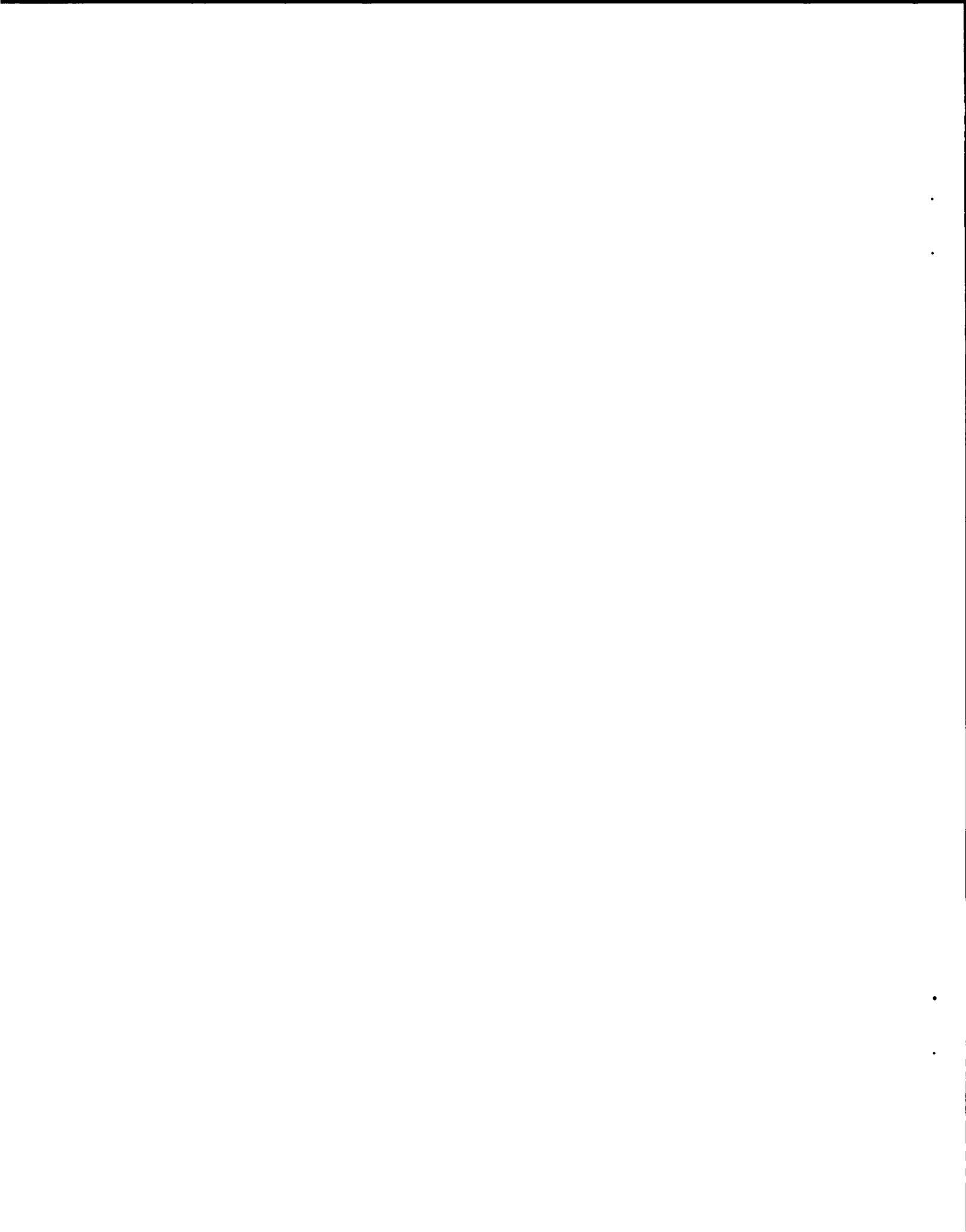
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Hydrogen, Deuterium, or Tritium Atoms

by

Gerald G. Ohlsen





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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.

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 Schroedinger 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

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

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:

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

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

$$i\hbar \dot{b}_{m_I, m_J} = [(\mu_0 g_J m_J + \mu_N g_I m_I) B_z + \alpha m_I m_J] b_{m_I, m_J} \quad (6)$$

$$\begin{bmatrix} \dot{b}_1 \\ \dot{b}_2 \\ \dot{b}_3 \\ \dot{b}_4 \end{bmatrix} = \frac{\mu_0 g_J}{i\hbar} \begin{bmatrix} \frac{1}{2}(1+k)B_z + \frac{1}{2}kB_0 & \frac{1}{2}kB_+ & 0 & \frac{1}{2}B_+ \\ \frac{1}{2}kB_- & \frac{1}{2}(1-k)B_z - \frac{1}{2}kB_0 & \frac{1}{2}B_+ & \frac{1}{2}B_0 \\ 0 & \frac{1}{2}B_- & -\frac{1}{2}(1+k)B_z + \frac{1}{2}kB_0 & \frac{1}{2}kB_- \\ \frac{1}{2}B_- & \frac{1}{2}B_0 & \frac{1}{2}kB_+ & -\frac{1}{2}(1-k)B_z - \frac{1}{2}kB_0 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix} \quad (8)$$

TABLE I

HYPERFINE STRUCTURE PARAMETERS

State	g_I	g_J	ϵ	B_1	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:

$$\begin{bmatrix} \dot{b}_1 \\ \dot{b}_2 \\ \dot{b}_3 \\ \dot{b}_4 \\ \dot{b}_5 \\ \dot{b}_6 \end{bmatrix} = \frac{\mu_0 g_J}{i\hbar} \begin{bmatrix} (\frac{1}{2}+k)B_z + \frac{1}{2}B_0 & kB_+ & 0 & 0 & 0 & 0 \\ kB_- & \frac{1}{2}B_z & kB_+ & 0 & 0 & 0 \\ 0 & kB_- & (\frac{1}{2}-k)B_z - \frac{1}{2}B_0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2}B_- & 0 & 0 \\ 0 & \frac{1}{2}B_- & B_0/\sqrt{2} & 0 & 0 & 0 \\ \frac{1}{2}B_- & B_0/\sqrt{2} & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \\ b_6 \end{bmatrix}, \quad (9)$$

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

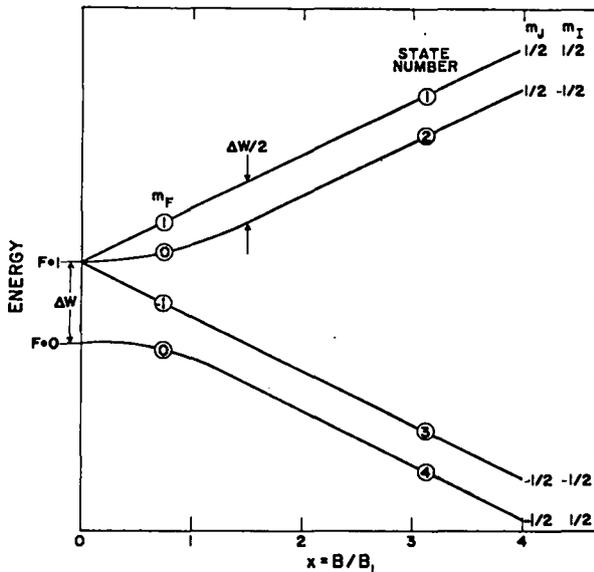


Fig. 1. Schematic Breit-Rabi diagram for 1S or 2S hydrogen or tritium atoms.

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

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

$$\begin{bmatrix} \dot{b}_1 \\ \dot{b}_2 \\ \dot{b}_3 \\ \dot{b}_4 \\ \dot{b}_5 \\ \dot{b}_6 \end{bmatrix} = \begin{bmatrix} 0 & 0 & \frac{1}{2}B_+ & 0 & 0 & 0 \\ 0 & \frac{1}{2}B_+ & B_0/\sqrt{2} & 0 & 0 & 0 \\ \frac{1}{2}B_+ & B_0/\sqrt{2} & 0 & 0 & 0 & 0 \\ -(\frac{1}{2}+k)B_z + \frac{1}{2}B_0 & kB_- & 0 & 0 & 0 & 0 \\ kB_+ & -\frac{1}{2}B_z & kB_- & 0 & 0 & 0 \\ 0 & kB_+ & -(\frac{1}{2}-k)B_z - \frac{1}{2}B_0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \\ b_6 \end{bmatrix}, \quad (9)$$

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-

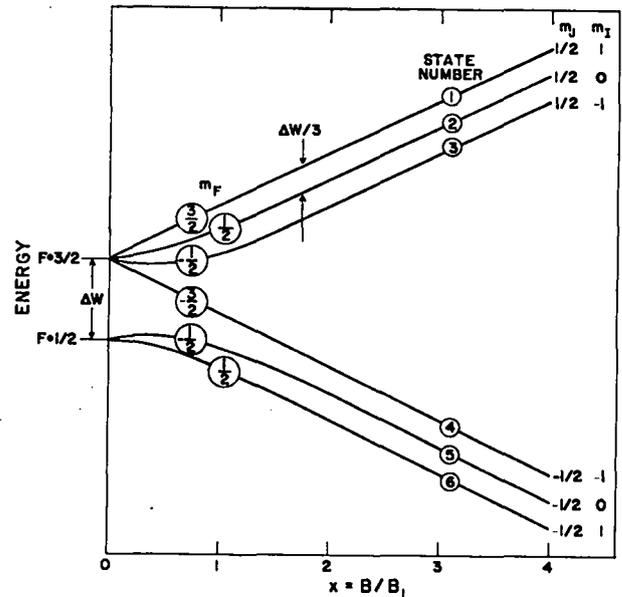


Fig. 2. Schematic Breit-Rabi diagram for 1S or 2S deuterium atoms.

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

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

$$\begin{bmatrix} b'_1 \\ b'_2 \\ b'_3 \\ b'_4 \\ b'_5 \\ b'_6 \end{bmatrix} = \begin{bmatrix} a_{++}c_{++} & a_{++}c_{+0} & a_{++}c_{+-} \\ a_{++}c_{0+} & a_{++}c_{00} & a_{++}c_{0-} \\ a_{++}c_{-+} & a_{++}c_{-0} & a_{++}c_{--} \\ a_{-+}c_{-+} & a_{-+}c_{-0} & a_{-+}c_{--} \\ a_{-+}c_{0+} & a_{-+}c_{00} & a_{-+}c_{0-} \\ a_{-+}c_{++} & a_{-+}c_{+0} & a_{-+}c_{+-} \end{bmatrix}$$

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

$$\begin{bmatrix} b_1'' \\ b_2'' \\ b_3'' \\ b_4'' \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \sqrt{\frac{1+\delta}{2}} & 0 & \sqrt{\frac{1-\delta}{2}} \\ 0 & 0 & 1 & 0 \\ 0 & -\sqrt{\frac{1-\delta}{2}} & 0 & \sqrt{\frac{1+\delta}{2}} \end{bmatrix} \begin{bmatrix} b_1' \\ b_2' \\ b_3' \\ b_4' \end{bmatrix}, \quad (18)$$

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

$$\begin{bmatrix} b_1'' \\ b_2'' \\ b_3'' \\ b_4'' \\ b_5'' \\ b_6'' \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \sqrt{\frac{1+\delta_+}{2}} & 0 & 0 & 0 & \sqrt{\frac{1-\delta_+}{2}} \\ 0 & 0 & \sqrt{\frac{1+\delta_-}{2}} & 0 & \sqrt{\frac{1-\delta_-}{2}} & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -\sqrt{\frac{1-\delta_-}{2}} & 0 & \sqrt{\frac{1+\delta_-}{2}} & 0 \\ 0 & -\sqrt{\frac{1-\delta_+}{2}} & 0 & 0 & 0 & \sqrt{\frac{1+\delta_+}{2}} \end{bmatrix} \begin{bmatrix} b_1' \\ b_2' \\ b_3' \\ b_4' \\ b_5' \\ b_6' \end{bmatrix}, \quad (19)$$

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

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

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

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

b) Deuterium Atoms

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

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

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

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	$P(\text{nuclear})$	$P(\text{electronic})$	
1	1	1	
2	$-\delta$	δ	
3	-1	-1	
4	δ	$-\delta$	
Deuterium Atoms			
State	$P_3(\text{nuclear})$	$P_{33}(\text{nuclear})$	$P(\text{electronic})$
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

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

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 $\beta_{\pm} = \sqrt{x^2+x+9/4}$. 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

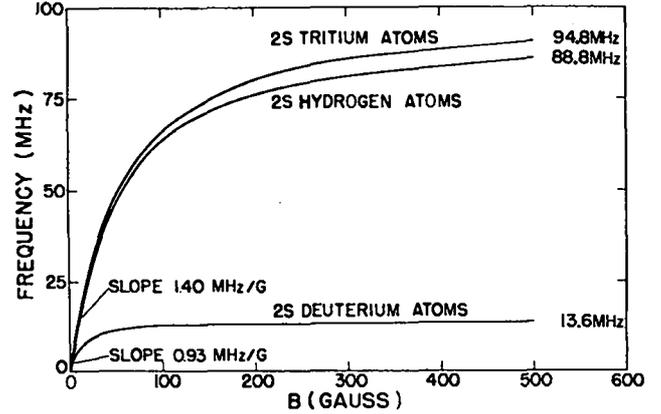


Fig. 3. Plot of the critical frequency for 2S tritium, hydrogen, and deuterium atoms versus magnetic field strength. For 1S atoms both the horizontal and vertical scales should be multiplied by 8.

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 $m_1 = 1$ 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

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

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

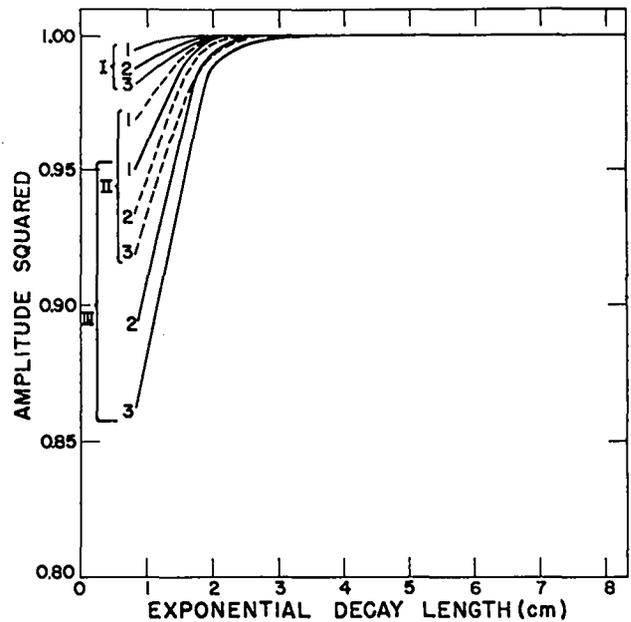


Fig. 4. Retained fraction of hydrogen atoms in state 1 (I), deuterium atoms in state 1 (II), and deuterium atoms in state 2 (III) for an exponentially shaped field which decays from 575 to 5 G. The abscissa is the "1/e" length Z . The curves marked 1, 2, and 3 correspond to particles which travel 1.25,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

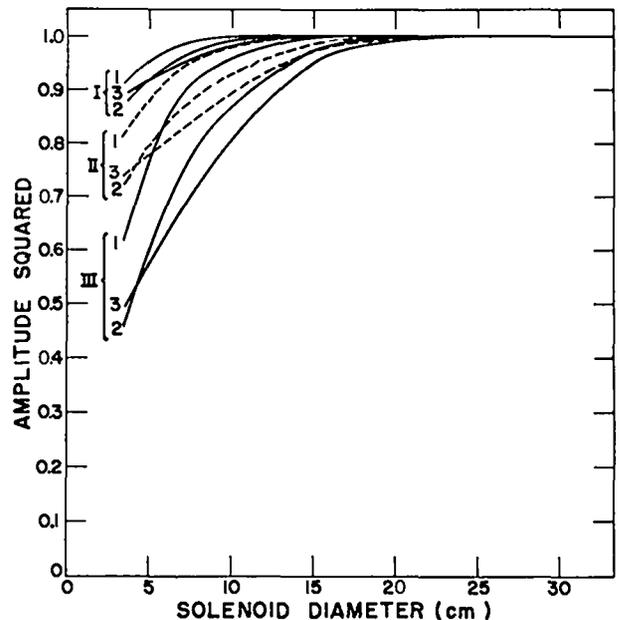


Fig. 5. Retained fraction of hydrogen atoms in state 1 (I), deuterium atoms in state 1 (II), and deuterium atoms in state 2 (III) for a particular axial field shape which can be achieved with a shielded solenoid (see Fig. 6). Curves are labeled as in Fig. 4. The abscissa refers to the diameter of the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

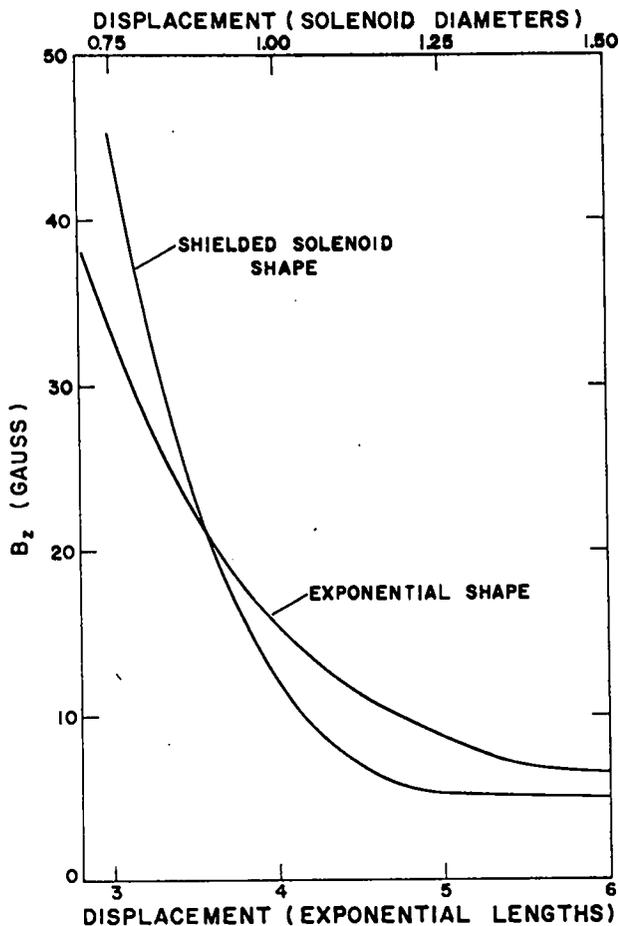


Fig. 6. Field shapes for the calculations whose results are presented in Figs. 4 and 5.

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 $B_z = 575 e^{-z/Z}$, $B_x = 5$. It is somewhat easier to induce depolarization in this case than in the case where the final field is longitudinal, because $\theta (= \tan^{-1} B_r/B_z)$ 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

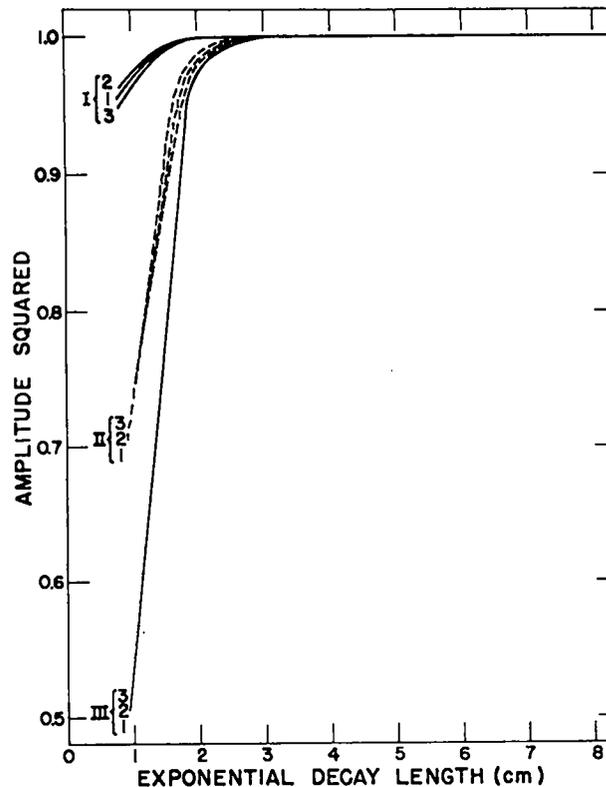


Fig. 7. Retained fraction of hydrogen atoms in state 1 (I), deuterium atoms in state 1 (II), and deuterium atoms in state 2 (III) for an exponentially declining axial field and a transverse final field. The curves and the abscissa are labeled as in Fig. 4. A velocity of 30 cm/usec is assumed.

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

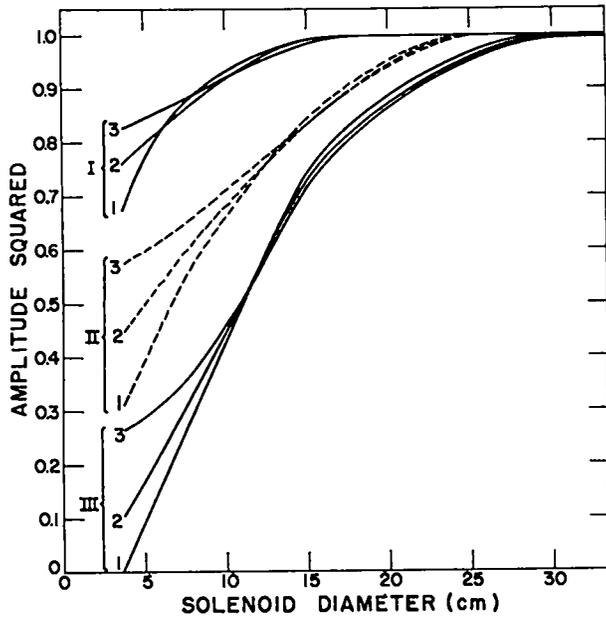


Fig. 8. Retained fraction of hydrogen atoms in state 1 (I), deuterium atoms in state 1 (II), and deuterium atoms in state 2 (III) for a particular axial field shape (see text) and a transverse final field. The curves and the abscissa are labeled as in Fig. 5. A velocity of 30 cm/ μ sec is assumed.

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

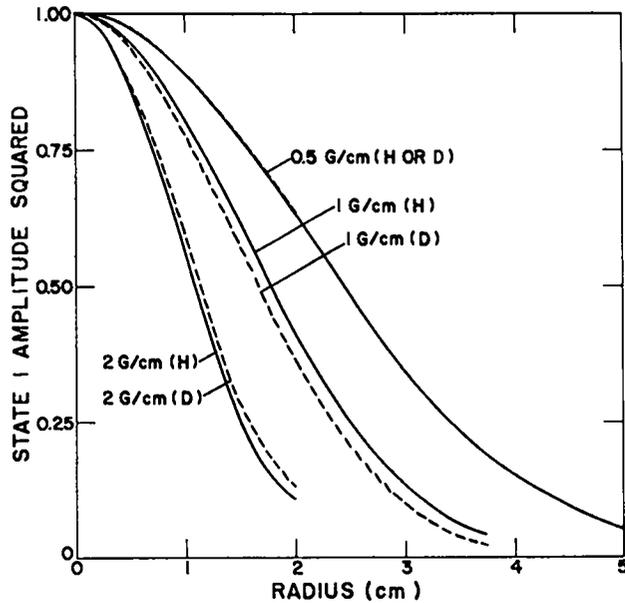


Fig. 9. Fraction of the initial state 1 making the desired transition when the field is linearly reversed at the indicated rate. The abscissa is the radius with respect to the (cylindrically symmetric) field axis. Slightly different results are obtained for hydrogen state 1 (H) and deuterium state 1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

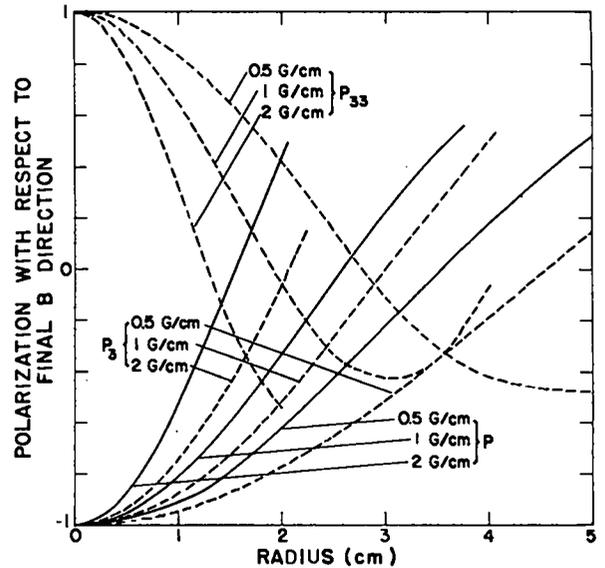


Fig. 10. Results of the calculations presented in Fig. 9 expressed in terms of P (for hydrogen) and P_3 and P_{33} (for deuterium). The polarizations are expressed with respect to the final field direction. A velocity of 30 cm/ μ sec is assumed.

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	$\frac{1}{\beta_+^2}[1-\cos(\frac{2\Delta W}{3\hbar})\beta_+ t]$	$-\frac{1}{\beta_+^2}[2x^2+2x+3/2+3\cos(\frac{2\Delta W}{3\hbar})\beta_+ t]$	
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 $\beta_{\pm} = (x^2 \pm x + 9/4)^{1/2}$. 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 $1 - (\frac{1}{9})^2$ 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.

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.

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

$$\mathcal{H} = H_0 + (\mu_0 g_J \vec{J} + \mu_N g_I \vec{I}) \cdot \vec{B} + a(\vec{I} \cdot \vec{J}),$$

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)
C  UNITS MICROSECONDS
COMMON/BL0CK1/A1, A2, A3, A4, C1, R0
COMMON/BL0CK2/RSQ(6, 201), TIME(201), BRX(201), BRV(201), BBZ(201),
1 P3(201), P33(201), PEL(201), N, I, TIME
COMMON/BL0CK3/M, NN
COMMON/BL0CK4/T1, T2, T3, T4, T5, T6, BZ1, BZ2, BRMAX, CPHI, SPHI, PI1, Y2, MODF,
1 VFLOC
COMMON/BL0CK5/DP/ZZ(100), BZZ(100), BRR(100), NZ
DIMENSION XO(30), XXP(30), BPLOT(201)
COMPLEX C1
1 FORMAT(10I6)
2 FORMAT(1H1)
3 FORMAT(* PROTONS      *6F14.8)
4 FORMAT(* NEUTERONS   *6F14.8)
5 FORMAT(* TRITONS     *6F14.8)
6 FORMAT(12F6.3)
7 FORMAT(* TIME          RX          BY          BZ          B          P3
1 P33          PFL          1          2          3          4          5
2 *)
8 FORMAT(14F9.4)
MJRNO010
MJRNO011
MJRNO012
MJRNO013
MJRNO014
MJRNO015
MJRNO016
MJRNO017
MJRNO018
MJRNO019
MJRNO020
MJRNO021
MJRNO022
MJRNO023
MJRNO024
MJRNO025
MJRNO026
MJRNO027
MJRNO028
MJRNO029
MJRNO030

```

```

9 FORMAT(6F12.6)
10 FORMAT(* STRONG FIELD STATE COEFFICIENTS, INITIAL COORDINATE SYSTEM
1M*)
11 FORMAT(* INTERMEDIATE FIELD STATE COEFFICIENTS, COORDINATE SYSTEM
1RATED S0 NEW Z AXIS POINTS ALONG FIELD DIRECTION *)
12 FORMAT(* P3=SQUARE, P33=PLUS, MAG FIELD PARAMS * 12F7.1)
13 FORMAT(* PARTICLE *I2,* STATF *I2,* INITIAL STRONG FIELD COEFFS *
11F6.3)
15 FORMAT(* Z(CM) THETA PHI BZ B P3
1 P33 PFL 1 2 3 4 5
2 A*)
READ 1,NZ
IF(NZ.EQ.0) GO TO 100
DO 90 I=1,NZ
READ 9,ZZ(I),BZZ(I),RRR(I)
90 PRINT9,ZZ(I),BZZ(I),RRR(I)
100 ITIME=0
PRINT 2
READ 1,M,NSTATE,MODE
PRINT 1,M,NSTATE,MODE
C M=1,2, OR 3 FOR PROTONS, DEUTERONS, OR TRITONS
C NSTATE= 1-4 OR 1-6 FOR INTERMEDIATE FIELD INITIAL STATES
C NSTATE= 11-14 OR 11-16 FOR STRONG FIELD STATES
C MODE=1,2, OR 3 DEPENDING ON BFIELD OPTION (SEE COMMENTS IN BFIFLD)
READ 9,TF,HHP
PRINT 9,TF,HHP
CALL SETUPB
CALL BFIFLD(TI,BRX(1),BRY(1),RBZ(1))
HTOT=SQRT(BRX(1)**2+BRY(1)**2+BBZ(1)**2)
A1PHA=0.0
HETA=-(3.1415927/180.0)*ARCTAN(SQRT(BRX(1)**2+BRY(1)**2),RBZ(1))
GAMMA=-(3.1415927/180.0)*ARCTAN(BRY(1),BRX(1))
DO 99 I=1,12
99 XN(I)=0.0
IF(M=2)101,102,103
101 HN=63.448/1.001522
A1=0.5*(1.0+n.001522/1.0n1522)
A2=0.5*(1.0-n.001522/1.0n1522)
A3=0.5*n.001522/1.001522
A4=0.0
N=4
PRINT 3,A1,A2,A3,A4,R0
X=HTOT/63.448
98 IF(NSTATE.GE.11) GO TO 144
DPLUS=SQRT(0.5+0.5*X/SQRT(1.0+X**2))
DMINUS=SQRT(0.5-0.5*X/SQRT(1.0+X**2))
GO TO (150,151,152,153),NSTATE
150 XN(1)=1.0
GO TO 104
151 XN(3)=DPLUS
XN(7)=DMINUS
GO TO 104
152 XN(5)=1.0
GO TO 104
153 XN(3)=-DMINUS
XN(7)=DPLUS
GO TO 104
154 NSTATE=NSTATE-10
XN(2*NSTATE-1)=1.0
GO TO 104
102 HN=14.605/1.000233
R0=(2.0/3.0)*BN
A1=0.5+0.000233/1.000233
A2=0.5-0.000233/1.000233
A3=0.000233/1.000233
A4=SQRT(0.5)
N=6
PRINT 4,A1,A2,A3,A4,R0
X=HTOT/14.605
IF(NSTATE.GE.11) GO TO 144
DPLUS=(X+.0/3.0)/SQRT(1.0+2.0*X/3.0+X**2)
DMINUS=(X-1.0/3.0)/SQRT(1.0-2.0*X/3.0+X**2)

```

```

        GO TO (140,141,142,143,144,145),NSTATE
140 X(1)=1.0
    GO TO 104
141 X(3)=SQRT(0.5+0.5*DPLUS)
    X(11)=SQRT(0.5-0.5*DPLUS)
    GO TO 104
142 X(5)=SQRT(0.5+0.5*DMINUS)
    X(9)=SQRT(0.5-0.5*DMINUS)
    GO TO 104
143 X(7)=1.0
    GO TO 104
144 X(5)=-SQRT(0.5-0.5*DMINUS)
    X(9)=SQRT(0.5+0.5*DMINUS)
    GO TO 104
145 X(3)=-SQRT(0.5-0.5*DPLUS)
    X(11)=SQRT(0.5+0.5*DPLUS)
    GO TO 104
146 NSTATE=NSTATE-10
    X(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 A0G=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(N,ALPHA,BETA,GAMMA,XD)
    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=ITIME
    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))
        THETA=ARCTAN(SQRT(BBY(I)**2+BBX(I)**2),BBZ(I))
        PRINT 8,POSN,THETA,PHIF,BBZ(I),BTOT,P3(I),P33(I),PEL(I),(BSQ(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,TT,TTF,1.0,0.0)
    CALL DLNL(10,10)
    CALL SLLIN(10,01)
    CALL SRLIN(10,02)

```

```

MJRN0103
MJRN0104
MJRN0105
MJRN0106
MJRN0107
MJRN0108
MJRN0109
MJRN0110
MJRN0111
MJRN0112
MJRN0113
MJRN0114
MJRN0115
MJRN0116
MJRN0117
MJRN0118
MJRN0119
MJRN0120
MJRN0121
MJRN0122
MJRN0123
MJRN0124
MJRN0125
MJRN0126
MJRN0127
MJRN0128
MJRN0129
MJRN0130
MJRN0131
MJRN0132
MJRN0133
MJRN0134
MJRN0135
MJRN0136
MJRN0137
MJRN0138
MJRN0139
MJRN0140
MJRN0141
MJRN0142
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MJRN0144
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MJRN0146
MJRN0147
MJRN0148
MJRN0149
MJRN0150
MJRN0151
MJRN0152
MJRN0153
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MJRN0155
MJRN0156
MJRN0157
MJRN0158
MJRN0159
MJRN0160
MJRN0161
MJRN0162
MJRN0163
MJRN0164
MJRN0165
MJRN0166
MJRN0167
MJRN0168
MJRN0169
MJRN0170
MJRN0171
MJRN0172
MJRN0173
MJRN0174

```

```

Dn 120 J=1,N
Dn 121 I=1,NTIME
121 HPLOT(I)=RSQ(J,I)
120 CALL PLOT(NTIME,TIME(1),I,BPLOT(1),1,44,1)
CALL DGA(50,950,50,500,T,TTF,1,0,-2,0)
CALL SRLIN(6,01)
CALL PLOT(NTIME,TIME(1),I,P33(1),1,16,0)
CALL PLOT(NTIME,TIME(1),I,P3(1),1,63,0)
CALL LINCNT(60)
PHI=PHI*1A0,0/3,1415927
WRITE(12,12)Z1,Z2,Z3,Z4,Z5,Z6,BZ1,BZ2,BRMAX,YI,PHI,VELOC
WRITE(12,13)M,NSTATE,(XO(I),I=1,NN)
CALL AOV(1)
PRINT 13,M,NSTATE,(XO(I),I=1,NN)
GO TO 100
END

```

MJRN0175
MJRN0176
MJRN0177
MJRN0178
MJRN0179
MJRN0180
MJRN0181
MJRN0182
MJRN0183
MJRN0184
MJRN0185
MJRN0186
MJRN0187
MJRN0188
MJRN0189
MJRN0190

```

SUBROUTINE SETUPR
C READS IN FIELD PARAMETERS AND COMPUTES SOME FREQUENTLY USED QUAN-
C TITIES FOR USE BY SUBROUTINE BFIELD
COMMON/BFIELD/T1,T2,T3,T4,T5,T6,BZ1,BZ2,BRMAX,CPHI,SPHI,PI2,Y2,MODE
1VFLOC
C DISTANCES IN CM FOR FIELD PARAMETER ENTRY
2 FORMAT(6F)2,6)
PI2=3.1415927/2,0
READ 2,B1,BZ2,BRMAX,Y1,PHI,VELOC
PRINT2,BZ1,BZ2,BRMAX,Y1,PHI,VELOC
READ 2,Z1,Z2,Z3,Z4,Z5,Z6
PRINT2,Z1,Z2,Z3,Z4,Z5,Z6
T1=Z1/VELOC
T2=Z2/VELOC
T3=Z3/VELOC
T4=Z4/VELOC
T5=Z5/VELOC
T6=Z6/VELOC
C Y1 IN CM, PH1 IN DEGREES
CPHI=COS(PHI*PI2/90,0)
SPHI=SIN(PHI*PI2/90,0)
GO TO(100,200,300),MODE
100 Y2=Y1
RETURN
200 Y2=-(Y1/2,0)*PI2*(BZ1-BZ2)/(VELOC*(T2-T1))
RETURN
300 Y2=(BZ1-BZ2)*Y1/(2,0*VELOC*(T2-T1))
RETURN
END

```

SETB0010
SETB0011
SETB0012
SETB0013
SETB0014
SETB0015
SETB0016
SETB0017
SETB0018
SETB0019
SETB0020
SETB0021
SETB0022
SETB0023
SETB0024
SETB0025
SETB0026
SETB0027
SETB0028
SETB0029
SETB0030
SETB0031
SETB0032
SETB0033
SETB0034
SETB0035
SETB0036
SETB0037
SETB0038

```

SUBROUTINE BFIELD(T,BX,BY,BZ)
C COMPUTES FIELD COMPONENTS AT POSITION Z=VELOC*T, Y=Y1, X=0
COMMON/BFIELD/T1,T2,T3,T4,T5,T6,BZ1,BZ2,BRMAX,CPHI,SPHI,PI2,Y2,MODE
1VFLOC
COMMON/BFIELD/ZZ(100),BZZ(100),BRR(100),NZ
GO TO(200,300,400),MODE
C MODE 1 (READ IN TABLES OF BZ,BR)
200 IF(T.GT.T1) GO TO 100
BY=BZ1
BY=0,0
BY=0,0
GO TO 500
100 IF(T.GT.T2) GO TO 101
Z=VELOC*T
C TABLE IN GAUSS ON AXIS AND 1 CM OFF AXIS NORMALIZED TO UNITY BZ(1)
CALL TABLE(Z,ZZ(1),NZ,I,MFLAG)
DBZDZ=(BZ(I+1)-BZ(I))/(ZZ(I+1)-ZZ(I))
DBRDZ=(BR(I+1)-BR(I))/(ZZ(I+1)-ZZ(I))
B7NORM=BZ(I)+DBZDZ*(Z-Z(I))
B8NORM=BR(I)+DBRDZ*(Z-Z(I))

```

BFLD0010
BFLD0011
BFLD0012
BFLD0013
BFLD0014
BFLD0015
BFLD0016
BFLD0017
BFLD0018
BFLD0019
BFLD0020
BFLD0021
BFLD0022
BFLD0023
BFLD0024
BFLD0025
BFLD0026
BFLD0027
BFLD0028
BFLD0029

```

      H7=BZ2+(H71-HZ2)*RZNORM
C  INITIAL RAY DEFINES Y-Z PLANE
      BY=Y2*(RZ1-HZ2)*RRNORM
      HX=0.0
      GO TO 500
101  H7=BZ2
      HV=0.0
      HY=0.0
      GO TO 500
C  MODE 2 (COSINE-SQUARED FIELD DECAY)
300  IF (T.GT.T1) GO TO 301
      HV=0.0
      HY=0.0
      H7=BZ1
      GO TO 500
301  IF (T.GT.T2) GO TO 302
      ARG=PI2*(T-T1)/(T2-T1)
      H7=BZ2+(BZ1-HZ2)*COS(ARG)**2
      BY=Y2*SIN(2.0*ARG)
      HV=0.0
      GO TO 500
302  HX=0.0
      HV=0.0
      H7=BZ2
      GO TO 500
C  MODE 3 (EXPONENTIAL FIELD DECAY)
400  IF (T.GT.T1) GO TO 401
      HX=0.0
      HV=0.0
      H7=BZ1
      GO TO 500
401  EARG=EXP(-(T-T1)/(T2-T1))
      H7=(RZ1-HZ2)*EARG+BZ2
      HV=0.0
      HY=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
      HD=0.0
      GO TO 505
501  IF (T.GT.T4) GO TO 502
      HQ=BRMAX*SIN(PI2*(T-T3)/(T4-T3))**2
      GO TO 505
502  HD=BRMAX
505  HY=HR*SPHT+BY
      BY=BR*CPHT+HX
      RETURN
      END

```

```

RFLD0030
RFLD0031
RFLD0032
RFLD0033
RFLD0034
RFLD0035
RFLD0036
RFLD0037
RFLD0038
RFLD0039
RFLD0040
RFLD0041
RFLD0042
RFLD0043
RFLD0044
RFLD0045
RFLD0046
RFLD0047
RFLD0048
RFLD0049
RFLD0050
RFLD0051
RFLD0052
RFLD0053
RFLD0054
RFLD0055
RFLD0056
RFLD0057
RFLD0058
RFLD0059
RFLD0060
RFLD0061
RFLD0062
RFLD0063
RFLD0064
RFLD0065
RFLD0066
RFLD0067
RFLD0068
RFLD0069
RFLD0070
RFLD0071
RFLD0072
RFLD0073
RFLD0074
RFLD0075
RFLD0076
RFLD0077
RFLD0078

```

```

      SUBROUTINE DERIV(T,V,FD)
C  COMPUTES THE FIRST DERIVATIVE OF THE STATE VECTOR FOR USE BY INTEG
      DIMENSION V(30),FD(30)
      COMMON/BLCK1/A1,A2,A3,A4,C1,R0
      COMMON/BLCK3/M,N,N
      COMPLEX B1,B2,B3,B4,B5,B6,BPLUS,BMINUS,C1,BDOT
      CALL BFIELD(T,AX,AY,AZ)
      BPLUS=CMPLX(X(AX),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=DFLTAW/(MII*GJ)      C1=MII*GJ/(HBAR*TI)  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)

```

```

DERI0010
DERI0011
DERI0012
DERI0013
DERI0014
DERI0015
DERI0016
DERI0017
DERI0018
DERI0019
DERI0020
DERI0021
DERI0022
DERI0023
DERI0024
DERI0025
DERI0026
DERI0027
DERI0028
DERI0029

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```

HNDOT=C1*(A3*RMINIUS*B1+(A2*BZ-0.25*B0)*B2+0.5*BPPLUS*B3+0.5*B0*B4) DERI0030
FN(3)=REAL(HNDOT) DERI0031
FN(4)=AIMAG(HNDOT) DERI0032
HNDOT=C1*(0.5*BMINIUS*B2+(0.25*B0-A1*BZ)*B3+A3*RMINUS*B4) DERI0033
FN(5)=REAL(HNDOT) DERI0034
FN(6)=AIMAG(HNDOT) DERI0035
HNDOT=C1*(0.5*RMINIUS*B1+0.5*B0*B2+A3*BPPLUS*B3-(A2*BZ+0.25*B0)*B4) DERI0036
FN(7)=REAL(HNDOT) DERI0037
FN(8)=AIMAG(HNDOT) 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 H0=DFLTAW/(1.5*MU*GJ) C1=MH*GJ/(HBAR*Y) UNITS 1/MICROSECOND DERI0043
R1=CMPLX(V(1),V(2)) DERI0044
R2=CMPLX(V(3),V(4)) DERI0045
R3=CMPLX(V(5),V(6)) DERI0046
R4=CMPLX(V(7),V(8)) DERI0047
R5=CMPLX(V(9),V(10)) DERI0048
R6=CMPLX(V(11),V(12)) DERI0049
HNDOT=C1*(A1*R7+0.5*B0)*R1+A3*BPPLUS*R2+0.5*BPPLUS*B6) DERI0050
FN(1)=REAL(HNDOT) DERI0051
FN(2)=AIMAG(HNDOT) DERI0052
HNDOT=C1*(A3*RMINIUS*B1+0.5*BZ*B2+A3*BPPLUS*B3+0.5*BPPLUS*B5+A4*B0*B4) DERI0053
FN(3)=REAL(HNDOT) DERI0054
FN(4)=AIMAG(HNDOT) DERI0055
HNDOT=C1*(A3*RMINIUS*B2+(A2*BZ-0.5*B0)*R3+0.5*BPPLUS*B4+A4*B0*B5) DERI0056
FN(5)=REAL(HNDOT) DERI0057
FN(6)=AIMAG(HNDOT) DERI0058
HNDOT=C1*(0.5*RMINIUS*B3+(0.5*B0-A1*BZ)*B4+A3*BMINIUS*B5) DERI0059
FN(7)=REAL(HNDOT) DERI0060
FN(8)=AIMAG(HNDOT) DERI0061
HNDOT=C1*(0.5*RMINIUS*B2+A4*B0*B3+A3*BPPLUS*B4-0.5*BZ*B5+A3*RMINUS*
1B6) DERI0062
FN(9)=REAL(HNDOT) DERI0063
FN(10)=AIMAG(HNDOT) DERI0064
HNDOT=C1*(0.5*BMINIUS*B1+A4*B0*B2+A3*BPPLUS*B5-(A2*BZ+0.5*B0)*B6) DERI0065
FN(11)=REAL(HNDOT) DERI0066
FN(12)=AIMAG(HNDOT) DERI0067
RETURN DERI0068
END) DERI0069
DERI0070

SUBROUTINE PRINT(T,VS) PRNT0010
C PRINTS STRONG FIELD SQUARED AMPLITUDES WITH RESPECT TO PROBLEM DE- PRNT0011
C FINE) Z AXIS. STORES WEAK FIELD SQUARED AMPLITUDES WITH RESPECT PRNT0012
C TO INSTANTANEOUS R AXIS FOR LATER PRINTOUT BY MAIN PROGRAM PRNT0013
COMMON/BLCK2/RSQ(6,201),TIME(201),BRX(201),BRY(201),BBZ(201),
1P3(201),P33(201),DEL(201),N*ITIME PRNT0014
COMMON/BLCK3/M,NN PRNT0015
DIMENSION V(12),VS(12),BRSQ(6) PRNT0016
ITIME=ITIME+1 PRNT0017
DO 90 I=1,NN PRNT0018
90 V(I)=VS(I) PRNT0019
CALL RENORM(V,VV) PRNT0020
IF(VV.GT.1.01) PRINT 80 PRNT0021
80 FORMAT(* RENORMALIZATION EXCEEDS 1 PERCENT*) PRNT0022
CALL BFIELD(T,BX,BY,BZ) PRNT0023
BRX(ITIME)=BX PRNT0024
BRY(ITIME)=BY PRNT0025
BRZ(ITIME)=BZ PRNT0026
RTOT=SQRT(BX**2+BRY**2+BBZ**2) PRNT0027
A1 PHA=13.1415927/180.0)*ARCTAN(BY,BX) PRNT0028
BETA=(3.1415927/180.0)*ARCTAN(SQRT(BX**2+BRY**2),BZ) PRNT0029
GAMMA=0.0 PRNT0030
GO TO (101,102,103),M PRNT0031
101 X=RTOT/63.448 PRNT0032
98 BPPLUS=SQRT(0.5+0.5*X/SQRT(1.0+X**2)) PRNT0033
BMINIUS=SQRT(0.5-0.5*X/SQRT(1.0+X**2)) PRNT0034
DO 105 I=1,4 PRNT0035
105 BRSQ(I)=V(2*I-1)**2+V(2*I)**2 PRNT0036
PRNT0037

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PPEL=BBSV(1)+BBSQ(2)-BBSQ(3)-BBSQ(4) PRNT003A
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 PRNT003B
P7Z=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(ITIME)=0.0 PRNT0043
P3(ITIME)=07 PRNT0044
HSQ(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))**2 PRNT0046
1*2 PRNT0047
HSQ(3,ITIME)=V(5)**2+V(6)**2 PRNT0048
HSQ(4,ITIME)=(-DMINUS*V(7)+DPLUS*V(8))**2+(-DMINUS*V(4)+DPLUS*V(8))**2 PRNT0049
1)**2 PRNT0050
PFL(ITIME)=HSQ(1,ITIME)+BSQ(2,ITIME)-HSQ(3,ITIME)-BSQ(4,ITIME) PRNT0051
GO TO 110 PRNT0052
102 X=HTOT/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=BBSV(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
P7Z=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
Q77=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(ITIME)=0Z PRNT0072
P33(ITIME)=0ZZ PRNT0073
HSQ(1,ITIME)=V(1)**2+V(2)**2 PRNT0074
HSQ(2,ITIME)=(E1*V(3)+E2*V(11))**2+(E1*V(4)+E2*V(12))**2 PRNT0075
HSQ(3,ITIME)=(E3*V(5)+E4*V(9))**2+(E3*V(6)+E4*V(10))**2 PRNT0076
HSQ(4,ITIME)=V(7)**2+V(8)**2 PRNT0077
HSQ(5,ITIME)=(-E4*V(5)+E3*V(9))**2+(-E4*V(6)+E3*V(10))**2 PRNT0078
HSQ(6,ITIME)=(-E2*V(3)+E1*V(11))**2+(-E2*V(4)+E1*V(12))**2 PRNT0079
PFL(ITIME)=HSQ(1,ITIME)+BSQ(2,ITIME)+HSQ(3,ITIME)-BSQ(4,ITIME) PRNT0080
1=HSQ(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,RX,RY,RZ,BTOT,PZ,P7Z,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,CMO, ROT 0016
ICMM 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)=CMP(X(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))
ww(3)=AMP*(AMP*VV(1)+AMM*VV(2)+AMM*(AMM*VV(3)+AMP*VV(4))
ww(4)=AMP*(APP*VV(1)+APM*VV(2)+AMM*(APM*VV(3)+APP*VV(4))
Dn 12 I=1.4
v(2*I-1)=REAL(ww(I))
12 v(2*I)=AIMAG(ww(I))
RETURN
20 CnS=COS(ETA)
SINB=SIN(ETA)
CnP=(0.5+n.5*CnS)*CEXP(-XI*(ALPHA+GAMMA))
CpO=(SINH/SQRT(2.0))*CEXP(-XI*GAMMA)
CpM=(0.5-n.5*CnS)*CEXP(XI*(ALPHA-GAMMA))
CnP=(-SINH/SQRT(2.0))*CEXP(-XI*ALPHA)
CnO=COSH
CnM=-CONJG(CnP)
CpP=CONJG(CpM)
CpO=-CONJG(CpO)
CpM=CONJG(CpP)
Dn 21 I=1.6
21 vv(I)=CMP1 X(v(2*I-1)*v(2*I))
ww(1)=APP*(CnP*VV(1)+CpO*VV(2)+CpM*VV(3)+APM*(CpM*VV(4)+CnO*VV(5)
1+CpP*VV(6))
ww(2)=APP*(CnP*VV(1)+CpO*VV(2)+CpM*VV(3)+APM*(CnM*VV(4)+CnO*VV(5)
1+CpP*VV(6))
ww(3)=APP*(CpM*VV(1)+CpO*VV(2)+CpM*VV(3)+APM*(CMM*VV(4)+CpO*VV(5)
1+CpP*VV(6))
ww(4)=AMP*(CpM*VV(1)+CpO*VV(2)+CpM*VV(3)+AMM*(CMM*VV(4)+CpO*VV(5)
1+CpP*VV(6))
ww(5)=AMP*(CnP*VV(1)+CpO*VV(2)+CpM*VV(3)+AMM*(CnM*VV(4)+CnO*VV(5)
1+CpP*VV(6))
ww(6)=AMP*(CpP*VV(1)+CpO*VV(2)+CpM*VV(3)+AMM*(CpM*VV(4)+CpO*VV(5)
1+CpP*VV(6))
Dn 22 I=1.6
v(2*I-1)=REAL(ww(I))
22 v(2*I)=AIMAG(ww(I))
RETURN
END

```

```

SUBROUTINE RENORM(N,V,VV)
C RENORMALIZES TO REMOVE ACCUMULATED DEVIATION FROM UNITY TOTAL
C PROBABILITY
DIMENSION V(12)
NN=2*N
VV2=0.0
Dn 10 I=1,NN
10 vv2=vv2+v(2*I-1)**2+v(2*I)**2
vv=sqrt(vv2)
Dn 11 I=1,NN
11 v(I)=v(I)/vv
RETURN
END

```

```

FUNCTION ARCTAN(Y,X)
C ARCTANGENT ROUTINE, CORRECT IN ALL QUADRANTS, IN DEGREES
IF(X)300,301,302
300 IF(Y)303,304,304
303 ARCTAN=ATAN(Y/X)-3.1415927
GO TO 311
304 ARCTAN=ATAN(Y/X)+3.1415927
GO TO 309
301 IF(Y)305,306,307
305 ARCTAN=-3.1415927/2.0
GO TO 308
306 ARCTAN=0.0
GO TO 308
307 ARCTAN=3.1415927/2.0
GO TO 308
302 ARCTAN=ATAN(Y/X)

```

```

308 ARCTAN=ARCTAN*180.0/3.1415927
RETURN
END

```

```

ACTN0026
ACTN0027
ACTN0028

```

```

SUBROUTINE TABLE (Z,ZZ,N7,I,MFLAG)
C RETURNS INDEX J OF NEXT SMALLER ENTRY OF ZZ(I)
C MFLAG=0 IF Z=ZZ(I) FOR SOME I
  DIMENSION ZZ(100)
  N,J=10
  MFLAG=1
  IF(Z.LT.Z7(1)) GO TO 30
  IF(Z.GT.Z7(N7)) GO TO 30
  DO 10 I=1,N7+10
  IF(Z.EQ.Z7(I)) MFLAG=0
  IF(Z.LT.Z7(1)) GO TO 20
10 CONTINUE
  N=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,TF,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 RUNGA-KUTTA METHOD
  LOGICAL ACC
  COMMON/INT/N,TF,H,H0,HP,M,VM,J,ACC,XLB,RELTST,ABSTST,FACTOR,BND,
  IX(30,5),F(30,5),F(30),XP(30),G(30,4),IDOUBL,NDOUBL
  DIMENSION X0(30),XP(30)
C SET UP INITIAL VALUES
  N=NN
  TF=TF
  H=HH
  HP=HHP
  M=MM
  VM=VVM
  DO 10 I=1,N
10 X(I,1)=X0(I)
  T=TI
  HND=TI+HP
  H=H
  ABSTST=ABS
  RELTST=REL
  FACTOR=RELTST/ABSTST
  XLR=0.005*RELTST
  IDOUBL=0
  NDOUBL=3
  H=2.0*H
30 CALL START(I,RETRN)
  GO TO (10,99),IRETRN
C SHOULD ANY OF THE STARTING VALUES BE PRINTED OUT
100 I=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(T,4)	INTE0051
	GO TO 30	INTE0052
50	CALL TEST(I,RETRN)	INTE0053
	GO TO (101,60),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	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)	STRTO010
C	RUNGA-KUNTA STARTING METHOD	STRTO011
	LOGICAL ACC	STRTO012
	COMMON/INT/N,T,TF,H,H0,HP,M,VM,J,ACC,XLB,RELT,ABSTST,FACTOR,BND,	STRTO013
	IX(30,5),F(30,5),F(30),XP(30),G(30,4),IDOUHL,NDUURL	STRTO014
	J=2	STRTO015
	CALL RNGA	STRTO016
10	DO 15 I=1,N	STRTO017
15	XP(I)=X(I,2)	STRTO018
C	XP(I)=DHL INTERVAL RESULT FOR ERROR ANALYSIS	STRTO019
	T=T+H	STRTO020
	H=0.5*H	STRTO021
	IF ((T+H),NE,T) GO TO 30	STRTO022
	PRINT 20	STRTO023
20	FORMAT(50H EQNS CANNOT BE SOLVED FURTHER WITHIN GIVEN ERROR)	STRTO024
	TDLUSH=T+H	STRTO025
	PRINT 21, TPLISH,T	STRTO026
21	FORMAT(6H T+H= E15.10, 6H T= E15.10)	STRTO027
	IRETRN=2	STRTO028
	RETURN	STRTO029
30	DO 40 J=2,3	STRTO030
40	CALL RNGA	STRTO031
41	CALL ACCRY	STRTO032
	IF (.NOT.ACC) GO TO 10	STRTO033
	J=4	STRTO034
	CALL RNGA	STRTO035
	IRETRN=1	STRTO036
	RETURN	STRTO037
	END	STRTO038

	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,RELT,ABSTST,FACTOR,BND,	RNGA0012
	IX(30,5),F(30,5),F(30),XP(30),G(30,4),IDOUHL,NDUURL	RNGA0013
	CALL DERIV(T,X(1,1-1),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(T,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(T,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(T,J-1)+G(I,3)	RNGA0026

```

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

      SUBROUTINE ACCRY
      LOGICAL ACC
      COMMON/INT/N,T,TF,H,H0,H0,M,VM,J,ACC,XLB,RELST,ABSTST,FACTOR,BND,
      1X(30,5),F(30,5),E(30),XP(30),G(30,4),IDOUHL,NDOURL
      ACC=.TRUE.
      DO 50 I=1,N
      E(I)=ABS(XP(I)-X(T,J))
      IF (E(I).GE.ABS(X(I,J))*RELST) GO TO 10
      E(I)=E(I)/ABS(X(I,J))
      GO TO 50
10 IF (E(I).GE.ABSTST) GO TO 20
      E(I)=E(I)*FACTOR
      GO TO 50
20 T=T-H
      H0=0.5*H
      ACC=.FALSE.
75 FORMAT(1H , 16HSTEP SIZE CUT TO, F12.8, 6H AT T=, F12.8)
      PRINT 75,H0,T
      GO TO 99
50 CONTINUE
99 RETURN
      END
      ACCY0010
      ACCY0011
      ACCY0012
      ACCY0013
      ACCY0014
      ACCY0015
      ACCY0016
      ACCY0017
      ACCY0018
      ACCY0019
      ACCY0020
      ACCY0021
      ACCY0022
      ACCY0023
      ACCY0024
      ACCY0025
      ACCY0026
      ACCY0027
      ACCY0028
      ACCY0029
      ACCY0030
      ACCY0031
      ACCY0032
      ACCY0033

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

```

```

J=2
H=HND*T
CALL RNGA
CALL PRINT(T,X(1,J))
HND=RND*HND
C RESTORE VARIABLES TO PROCEED
J=JSAVE
H=HSAVE
T=TSAVE
DO 45 I=1,N
X(I,1)=X1(I)
X(I,2)=X2(I)
F(I,1)=F1(I)
46 F(I,2)=F2(I)
50 IF (J.NF) GO TO 99
DO 60 I=1,N
X(I,4)=X(I,5)
DO 60 J=2,5
60 F(I,J-1)=F(I,J)
99 IDEFTRN=1
RETURN
END

```

TEST0045
TEST0046
TEST0047
TEST0048
TEST0049
TEST0050
TEST0051
TEST0052
TEST0053
TEST0054
TEST0055
TEST0056
TEST0057
TEST0058
TEST0059
TEST0060
TEST0061
TEST0062
TEST0063
TEST0064
TEST0065
TEST0066

```

SUBROUTINE DTIME
C FIND VALUE OF T WHERE THE M/T H VARIABLE REACHES THE VALUE VM
COMMON/INT/N,T,TF,H,H0,HP,M,VM,J,ACC,XLB,RELTST,ABSTST,FACTOR,RND,
IX(30,5),F(30,5),F(30),XP(30),G(30,4),IDOURL,NDOURL
ITIME=SIOW D(30)
YI=X(M,J)
Y0=X(M,J-1)
DFLT=-ABS(H*Y1/(Y1-Y0))
10 H=DELT
DO 20 I=1,N
20 X(I,1)=X(I,J)
J=2
CALL RNGA
CALL DERIV(T,X(1,I),D)
DELT=(VM-X(M,J))/D(M)
IF (ABS(DELT).GE.1.0E-4) GO TO 10
X(M,J)=VM
RETURN
END

```

DIOD0010
DIOD0011
DIOD0012
DIOD0013
DIOD0014
DIOD0015
DIOD0016
DIOD0017
DIOD0018
DIOD0019
DIOD0020
DIOD0021
DIOD0022
DIOD0023
DIOD0024
DIOD0025
DIOD0026
DIOD0027
DIOD0028

```

SUBROUTINE ADAMS
C INTEGRATE ONE STEP BY THE ADAMS PREDICTOR-CORRECTOR METHOD
COMMON/INT/N,T,TF,H,H0,HP,M,VM,J,ACC,XLB,RELTST,ABSTST,FACTOR,BND,
IX(30,5),F(30,5),F(30),XP(30),G(30,4),IDOURL,NDOURL
J=5
CALL DERIV(T,X(1,4),F(1,4))
DO 10 I=1,N
10 X(I)=X(I,4)+0.04166667*H*(55.0*F(I,4)-59.0*F(I,3)
+37.0*F(I,2)-9.0*F(I,1))
T=T+H
CALL DERIV(T,XP,F(1,5))
DO 20 I=1,N
20 X(1,5)=X(1,4)+0.04166667*H*(9.0*F(I,5)+19.0*F(I,4)
+5.0*F(I,3)+F(I,2))
RETURN
END

```

ADAM0010
ADAM0011
ADAM0012
ADAM0013
ADAM0014
ADAM0015
ADAM0016
ADAM0017
ADAM0018
ADAM0019
ADAM0020
ADAM0021
ADAM0022
ADAM0023
ADAM0024
ADAM0025

```

SUBROUTINE DOUBLE (IRETRN)
C TEST TO SEE IF INTERVAL CAN BE DOUBLED
COMMON/INT/N,T,TF,H,H0,HP,M,VM,J,ACC,XLB,RELTST,ABSTST,FACTOR,RND,
IX(30,5),F(30,5),F(30),XP(30),G(30,4),IDOURL,NDOURL
IDOURL=IDOURL*1

```

DBLE0010
DBLE0011
DBLE0012
DBLE0013
DBLE0014

```

      IF (INDOURL.LT.NDOURL) GO TO 99
C  ALLOWS DOUBLE ATTEMPT ONLY EVERY NDOURL/TH CALL
      INDOURL=0
      DO 10 I=1,N
      IF (E(I).GT.XLR)GO TO 99
10  CONTINUE
      U)=HR/(2.0*H)
      IF (D1.LE.2.0) GO TO 99
      U2=(XND-T)/(2.0*H)
      IF (D2.LE.2.0) GO TO 99
      DO 20 I=1,N
20  X(I+1)=X(I+4)
      HR=2.0*H
      H=2.0*HR
30  FORMAT(18H STEP INCREASED TO F12.8. 6H AT T= F12.8)
C  PRINT 30,10,T
      IRETN=2
      RETURN
99  IRETN=1
      RETURN
      END

```

```

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

```