Non-adiabatic spin transitions in metastable hydrogen

by Ralph Dale Hight

n A thesis submitted in partial fulfillment of the requirements for the degree of DOCTOR OF PHILOSOPHY in PHYSICS
Montana State University

Abstract:
We consider the problem of non-adiabatic passage of an oriented spin through an inhomogeneous magnetic field. Differential equations for the spin state amplitudes for an arbitrary magnetic field are derived for the two cases of spin 1/2 and spin 1. The field is shown to be completely characterized by a single parameter called the adiabaticity parameter α The adiabaticity parameter is the ratio of the field magnitude to the field rotation rate. By means of a pedagogical example, a criterion for defining regions of adiabaticity (no spin flips) and non-adiabaticity (spin flips) is developed.

Using this criterion, we define transition lengths for regions where transitions occur.

We solve the amplitude equations for a simple type of magnetic field and calculate the spin flip probability. The field is assumed constant everywhere except in a small region where the axial component goes linearly through zero, reversing its direction. We constructed a magnetic field that closely approximates the above field. By using the F = 1 hyperfine states in the 2S 1/2 level of atomic hydrogen, we confirm the theory by comparison with experiment.

From the experimentally verified theory; we propose a novel method of producing a beam of metastable (2S 1/2) atomic hydrogen polarized completely in the F = 1, mf = 0 hyperfine state.

NON-ADIABATIC SPIN TRANSITIONS IN METASTABLE HYDROGEN

By

RALPH DALE HIGHT

A thesis submitted in partial fulfillment
of the requirements for the degree

of

DOCTOR OF PHILOSOPHY

in

PHYSICS

APPROVED:

R. T. Robiscoe (5/24/75)
Chairman, Examining Committee

Head, Major Department

Graduate Dean

MONTANA STATE UNIVERSITY
Bozeman, Montana

May, 1975

ACKNOWLEDGMENTS

I would like to express my appreciation and gratitude to Dr. R. T. Robiscoe for suggesting this work and for his support during the dark times.

I wish to thank my dear wife for her unfailing support and patience.

I would like to thank Mr. Fred Blankenberg for his electronic wizardry and friendship.

To all the others both large and small who helped me either voluntarily or involuntarily, I thank you.

TABLE OF CONTENTS

			Page
Acknowledgements			iii
Table of Contents			iv
List of Tables			vi
List of Figures			vii
Chapter			
I.	Introduction		1
	1.	History and Interest	1
	2.	What is Non-adiabatic Spin Passage	3
	3.	Overview of the Experiment	10
II.	Theory		20
	1.	A Spin Flip Problem	20
	2.	Adiabaticity Parameter	28
	3.	Two Level Passage	37
	4.	Three Level Non-adiabatic Passage	43
	5.	Evolution Matrix	47
	6.	Velocity and Beam-size Averaging	67
	7.	Summary	73
III.	Experimental Apparatus		74
	1.	Overview	74
	2.	Beam Source	77
	3.	Excitation	79
	4.	Hyperfine State Analyzer	90
	5.	Detectors	99

Page

6. Flopper 111

7. Procedure 119

IV. Data and Conclusions 133

1. Flopper Curves 133

2. Time of Flight Spectra 153

3. Pure Polarized Beam 158

4. Conclusion 162

Appendices

I. Three Level Spin Flip Probability for Constant α 165

II. Lebeda's Computer Program for the Evolution Matrix 170

III. Three level β_B Initially Non-zero Spin Flip Probabilities 186

IV. Velocity and Beam Averaging Computer Fits 188

V. Quenching of the $2S_{\frac{1}{2}}$ Metastable State in Atomic Hydrogen 193

VI. Averaging over Velocity Window 197

VII. Magnetic Field of a Set of Opposing Solenoids 198

VIII. Uncertainty in the β_B Population 205

Footnotes 207

Bibliography 210

LIST OF TABLES

Table		Page
I.	Typical Alphatron Operating Conditions	78
II.	Various Machine Parameters	132
III.	Flopper Data Summary Table	142
IV.	TOF Spectra Data	159

LIST OF FIGURES

Figure		Page
1.	Diagram of a spin particle entering a magnetic field.	5
2.	Spin flip probability for a spin $+\frac{1}{2}$ versus adiabaticity parameter for a constant magnetic field rotating uniformly through 180 degrees.	9
3.	Zeeman diagram of the fine structure and hyperfine structure states in the $2S_{\frac{1}{2}}$ and $2P_{\frac{1}{2}}$ levels of atomic hydrogen.	12
4.	Non-velocity selected flopper curve showing the conversion percentage of β_B as a function of flopper current.	15
5.	Velocity selected flopper curves.	17
6.	A simple rotating magnetic field.	31
7.	The inverse adiabaticity parameter versus distance for the magnetic field in Figure 6.	35
8.	Two level spin flip probability for the adiabaticity parameter shown in Figure 7 as a function of magnetic field.	42
9.	Computer generated solutions (χ's) for the magnitudes of the elements of $\varepsilon(\pi,0)$ with their curve fitted analytic functions (solid lines).	55
10.	Computer generated phase.	57
11.	Three level spin flip probability versus magnetic field.	64
12.	Velocity and beam averaged three-level spin flip probability versus magnetic field.	72
13.	Alphatron diagram.	76
14.	Hydogen dissociation curve.	81

15. Pressure dependence of the fractional dissociation and metastable intensity. 83

16. Atomic hydrogen $2S_{\frac{1}{2}}$ excitation curve. 86

17. Quenchable signals as a function of e-gun collimating field. 88

18. β_B quench curve. 93

19. α quench curve. 95

20. Beam notch curve. 98

21. Lamb shift resonance curve. 101

22. Time of flight electronics diagram. 105

23. Typical time of flight spectrum with time mark. 107

24. Velocity selection electronics diagram. 109

25. Cross-section of flopper. 113

26. Magnetic fields for the flopper shown in Figure 25. 116

27. Spatial variation of the adiabaticity parameter: χ's are experimentally determined and solid lines are theoretical experimental. 118

28. Maximum non-adiabaticity for the second crossing point as a function of flopper current. 121

29. Magnitude and rotation angle for the magnetic field environment. 123

30. Oven temperature versus the peak position in the time of flight spectrum. 128

31. Gaussian curve fit to the time of flight spectrum. 131

32. Flopper curve I. 135

33. Flopper curve II. 137

34. Flopper curve III. 139

35. Velocity selected flopper curve. 141

36. Oscillations from flopper curve I. 145

37. Oscillations from flopper curve II 147

38. Oscillations from flopper curve III. 149

39. Period plot for the oscillations in Figures 36, 37, and 38. 152

40. Time of flight spectra for the β_B state. 155

41. Period plots of the oscillations in the time of flight spectra. 157

42. β_B state initially non-zero flopper curves. 161

43. Three level constant α spin flip probability. 169

44. Comparison of the approximate L-Z envelope with the computer integration. 190

45. Comparison of the damped oscillatory term approximation with the computer integration. 192

46. Flopper cross-section. 201

47. Flopper field configuration. 204

ABSTRACT

We consider the problem of non-adiabatic passage of an oriented spin through an inhomogeneous magnetic field. Differential equations for the spin state amplitudes for an arbitrary magnetic field are derived for the two cases of spin $\frac{1}{2}$ and spin 1. The field is shown to be completely characterized by a single parameter called the adiabaticity parameter α. The adiabaticity parameter is the ratio of the field magnitude to the field rotation rate. By means of a pedagogical example, a criterion for defining regions of adiabaticity (no spin flips) and non-adiabaticity (spin flips) is developed. Using this criterion, we define transition lengths for regions where transitions occur.

We solve the amplitude equations for a simple type of magnetic field and calculate the spin flip probability. The field is assumed constant everywhere except in a small region where the axial component goes linearly through zero, reversing its direction. We constructed a magnetic field that closely approximates the above field. By using the F = 1 hyperfine states in the $2S_{\frac{1}{2}}$ level of atomic hydrogen, we confirm the theory by comparison with experiment.

From the experimentally verified theory, we propose a novel method of producing a beam of metastable ($2S_{\frac{1}{2}}$) atomic hydrogen polarized completely in the F = 1, $m_F = 0$ hyperfine state.

CHAPTER I

INTRODUCTION

1.1 History and Interest

The problem of non-adiabatic passage of an oriented spin through an inhomogeneous magnetic field was studied in the 1930's for its potential importance in measurements of the magnitude and sign of nuclear magnetic moments.(1,2,3) Theories were developed by Majorana(4) and Guttinger(5), with extensions by Rabi(6), and Schwinger(7), and others(8). Experiments were performed by Stern(9) and Segrè(10). Only the gross aspects of the theory were tractable due to its complexity (no computers were available to solve the non-linear equations). The existing technology severely limited the experimental investigations.

The situation was soon remedied if not clarified by the rapid development of molecular beam magnetic resonance methods. The theory of these experiments was easier to handle and yielded far more information than could be expected from non-adiabatic passage work. Non-adiabatic transitions, sometimes called "spin flips" or "Majorana flops," were then relegated to the status of a simple warning to all atomic and molecular physicists: namely, avoid them, for they are not well understood, and they will at best depolarize a beam of oriented spins.(11,12)

Very little work on Majorana flops was done until recently. An experiment(13), which used Majorana flops to selectively populate a particular spin state, found unexplained structure in the production curve for the spin state of interest. Since the major aim of that experiment was not the study of Majorana flops per se, the phenomena was merely noted and only a cursory treatment of the data was done. The problem of explaining this structure was left until 1970 when we began the work presented here.

The non-adiabatic passage of a beam of oriented spins through an inhomogeneous magnetic field is, in itself, of interest as an exercise in quantum mechanics. However, the problem can be related to the more general phenomena of scattering. In fact, the amplitude equations for charge exchange scattering are identical in structure[14,15] to the equations describing non-adiabatic passage. In most scattering experiments, any "structure" in the amplitudes, which is predicted by various approximate solutions, tends to be wiped out by a necessary averaging over the impact parameter and the velocity distribution of the beam. Thus, the validity of different approximations cannot be tested as long as the gross aspects of the scattering theories are similar. This suggests that a definitive study of non-adiabatic passage might provide a convenient and controllable analogue test for a variety of collision problems. In fact, various approximate theories developed for scattering problems can be checked in detail only if the strength and duration of the interaction can be controlled. This is possible, in principle, for a non-adiabatic passage experiment.

During the course of this study, a possible new method for the production of a completely polarized beam of neutral metastable hydrogen was discovered. We propose a method using Majorana flops directly, which is ironic in view of the usual warnings about the depolarizing properties of the Majorana flops.[11,12] Further work along this line is now being attempted, and results will be reported elsewhere.

1.2 What is Non-adiabatic Spin Passage?

An atom in a non-zero spin state, moving through an inhomogeneous magnetic field, is acted on by a time-varying field in the atom's rest frame. If the field variation is sufficiently slow, the adiabatic theorem predicts that the spin will remain aligned with the field and will not be "flipped" (i.e. will not make a transition to a different spin state). If, however, the field rotates at a rate on the order of the spin Larmor frequency, then there are Fourier components of the field near the spin flip resonance frequency. These Fourier components may be large enough to "flip" the spin. If spin flips occur, then the motion of the spin in the field is a "non-adiabatic passage."

An illustration of "spin-flips" may be given by considering a simple two-level problem.[16] The details of this two-level problem will be given in Chapter II and we will only discuss the highlights here.

Consider the entry of a polarized spin $\frac{1}{2}$ particle at a velocity $\vec{v}$ into a magnetic field $\vec{H}$ which is a function of position as shown in Figure 1. The spin interacts with the magnetic field through its

Figure 1: Diagram of a spin particle entering a magnetic field.

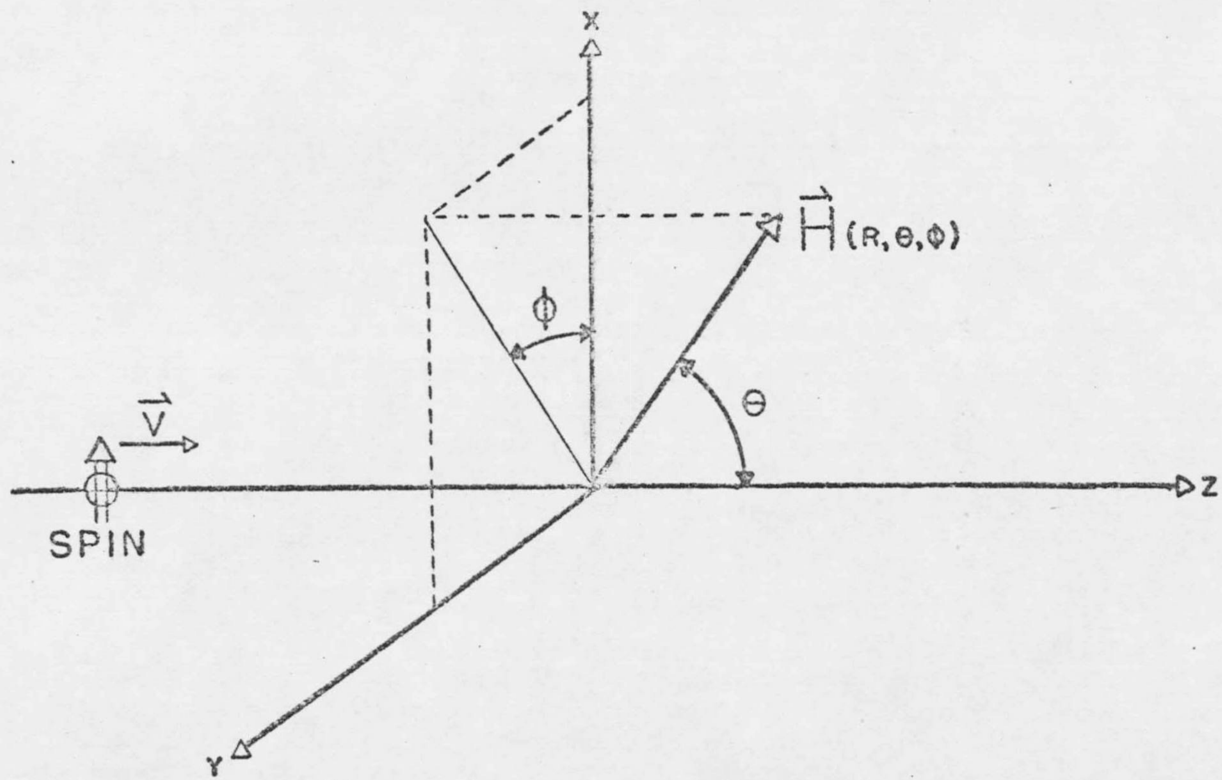

FIG. 1

magnetic moment $\vec{\mu}$, where $\vec{\mu} = \mu_B\hat{\sigma}$, $\hat{\sigma}$ are the Pauli spin matrices for a spin $\frac{1}{2}$ particle, and μ_B is the Bohr magneton. The spin Hamiltonian is then simply $\vec{\mu} \cdot \vec{H}$ and the spin wave function is

$$\psi(t) = a_1(t)\exp(-i\omega_1 t)\alpha_1 + \alpha_2(t)\exp(-i\omega_2 t)\alpha_2.$$

Here $\alpha_{1,2}$ are the spin-up and spin-down bispinors, respectively. Time-dependent perturbation theory then gives the equations of motion for the amplitudes $a_{1,2}(t)$. Defining the magnetic field in spherical polar coordinates and performing the unitary transformation $\mathbb{G}(t) = \mathbb{S}(t)\,\mathbb{B}(t)$, the equations of motion in matrix notation may be separated into an eigen-value term and a coupling term, as (1)

$$d\mathbb{B}/dt = -(i\omega(t)/2)\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\mathbb{B} - d\theta(t)/dt/2\begin{pmatrix} 0 & -\exp(-i\phi) \\ \exp(i\phi) & 0 \end{pmatrix}\mathbb{B}.$$

The Larmor frequency, $\omega(t)$, is defined as $\omega = (2\mu_B/\hbar)H(t)$ and $d\theta/dt$ is the magnetic field turning rate. In general, Equation (1) can not be solved explicitly. However, it is in a convenient form to discuss the asymptotic behavior when either ω or $d\theta/dt$ is much larger than the other. When $\omega \gg d\theta/dt$, we have weak coupling and do not really expect any spins to be appreciably flipped. On the other hand, when $d\theta/dt \gg \omega$, we expect a large number of spins to be flipped.

It will be convenient at this point to define the ratio of ω and $d\theta/dt$ as the "adiabaticity parameter": $\alpha(t) = \omega/(d\theta/dt)$. When $\alpha \gg 1$, the eigen-value matrix dominates ($\omega \gg d\theta/dt$). The approximate solutions for the $a(t)$ amplitudes with the initial conditions $a_1(0) = 1$, $a_2(0) = 0$, $d\theta/dt \sim 0$, and $\theta(\theta_0) = 0$ are simply: $|a_1(t)|^2 = 1$, and $|a_2(t)|^2 = 0$. This is known as adiabatic passage; and in fact, $\alpha \gg 1$ is one of the criteria used to design bending magnets for Stern-Gerlach type experiments. When $\alpha \ll 1$, the non-diagonal matrix dominates and for $a_1(0) = 1$, $a_2(0) = 0$, we have the final state amplitudes $a_1(t) = 1$ and $a_2(t) = 0$. However, now the magnetic field has changed directions while the spin has not; hence, there has been a spin flip. The spin did not follow the magnetic field rotation.

For a more specific example, consider the case of a constant magnitude magnetic field rotating uniformly from $\theta = 0$ to $\theta = \pi$. That is, α is a constant and the amplitude equations may be solved exactly. The spin flip probability from Chapter II is

$$P(\pi,\alpha) = \sin^2[\pi(1 + \alpha^2)^{\frac{1}{2}}/2]/(1 + \alpha^2) \quad . \tag{2}$$

As shown in Figure 2, for $\alpha \gg 1$, the probability of a spin-flip occurring is of order unity while for $\alpha \gg 1$, $P(\pi,\alpha)$ is close to zero. If a magnetic field is to be designed where less than 1% of the spins are flipped, a minimum value for α may be calculated by $P(\pi,\alpha) \ll 0.01$ ($\alpha \geq 10$). For most laboratory magnetic fields the parametric constant, α is not a "constant" but is a function of t or θ. We can however, estimate the approximate width of any non-adiabatic region. The calculation of any spin flip probability may be broken into regions of adiabatic passage, where the spin simply

Figure 2: Spin flip probability for a spin $\frac{1}{2}$ versus adiabaticity parameter for a constant magnetic field rotating uniformly through 180 degrees.