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ADVANCEMENTS IN NUCLEAR MAGNETIC RESONANCE, ELECTRON PARAMAGNETIC RESONANCE, MULTIPOLE MOMENTS, AND LIE GROUP PROPERTIES

by

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B.S. Kansas Wesleyan University, 2017

A dissertation submitted in partial fulfilment of the requirements for the degree of Doctor of Philosophy in Physics in the Department of Physics in the College of Sciences at the University of Central Florida
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Major Professor: Richard A. Klemm
ABSTRACT

To accurately solve the general nuclear spin state function in Nuclear Magnetic Resonance (NMR), a rotation wave approach was employed, allowing the reference frame to rotate in sync with the oscillating magnetic field. The spin state system was analogously treated as a Rubik’s Cube, ensuring the diagonalization of only the time-dependent part of the state function. Although Gottfried’s equation (1966) aligns with transitions between specific spin states $m$ and $m'$, his second rotation contradicts the conservation of angular momentum, resulting in inaccuracies for spin states with initial phase shifts or entangled states. Contrarily, Schwinger (1937) efficiently computed the coefficients for each spin state in a frequency range opposite to the Larmor frequency, using an unorthodox approach in quantum mechanics, which unfortunately led to the oversight of his work in subsequent citations.

This methodology was also applied to derive the general electron spin state function in Nuclear Magnetic Resonance (NMR) and Electron Paramagnetic Resonance (EPR), enabling the construction of a doubly rotated ground state for time-dependent perturbation theory. This was particularly relevant as the Hamiltonians for magnetic dipole, electric quadrupole, and magnetic octupole moments incorporate powers of $I \cdot J$ terms, necessitating the calculation of sub-state energy levels for perturbation, including those of molecules $^{14}\text{N}$ and $^{7}\text{Li}$.

Furthermore, the study expanded to the general Lie group for 3D rotations along three linearly independent axes, resulting in 12 distinct methods to achieve rotations in any arbitrary direction using these axes, yielding wave function with only one spin operator in each exponent.

The ongoing research is now concentrated on generating NMR spectra for $^{14}\text{N}$ in amino acids, furthering the understanding of nuclear spin dynamics in complex molecular systems.
To my family, friends, mentors, and all those who have never wavered in their pursuit of truth.
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# TABLE OF CONTENTS

LIST OF FIGURES ......................................................... xii

LIST OF TABLES ....................................................... xvii

CHAPTER 1: INTRODUCTION .............................................. 1

Stern-Gerlach Experiment ............................................. 1

NMR Machine History ................................................. 2

Definitions of Terms Relevant to NMR .............................. 4

The Relevant Techniques in NMR ..................................... 8

Multiple-Pulse Sequences ............................................. 8

Dilution ................................................................. 9

Magic-Angle Spinning .................................................. 10

Cross polarization ..................................................... 12

CHAPTER 2: LITERATURE REVIEW ................................. 13

Güttinger, 1931 .......................................................... 13

Majorana, 1932 .......................................................... 16
LIST OF FIGURES

Figure 1.1: Stern-Gerlach Experiment ................................. 2

Figure 1.2: Standard NMR Setting ........................................ 3

Figure 1.3: The Solution Type NMR Machine at the UCF the Office of Research .......................... 6

Figure 1.4: The Solid State NMR Machine at the UCF Physics Department and Sample .................. 7

Figure 1.5: A Basic Pulse Sequence ....................................... 8

Figure 1.6: The Magic Angle Spinning Setting ............................ 10

Figure 1.7: Magic Angle Spinning Example ............................... 12

Figure 3.1: The Process of Fixing a Rubik’s Cube .......................... 26

Figure 4.1: Spin I=1/2 .................................................... 51

Figure 4.2: Spin I=1 ..................................................... 52

Figure 4.3: Spin I=3/2 .................................................... 53

Figure 4.4: Spin I=2 ..................................................... 54

Figure 4.5: Spin \( I = 1/2 \) and \( 0.95 \leq \frac{\omega}{\omega_{n,e}^0} \leq 1.05 \) .................................................. 56

Figure 4.6: Spin \( I = 1/2 \) and \( 0.99 \leq \frac{\omega}{\omega_{n,e}^0} \leq 1.01 \) .................................................. 57
Figure 4.7: Spin \( I = \frac{1}{2} \) and \( 0.95 \leq \frac{\omega}{\omega_{n,e0}} \leq 1.05 \) The Probabilities of Spin States Crossing Each Other .............................................. 59

Figure 4.8: Spin \( I = \frac{1}{2} \) and \( 0.95 \leq \frac{\omega}{\omega_{n,e0}} \leq 1.05 \) Phase Affect \( (\pm) \) ................. 60

Figure 4.9: Spin \( I = 1 \) and \( 0.95 \leq \frac{\omega}{\omega_{n,e0}} \leq 1.05 \) ......................................................... 61

Figure 4.10: Spin \( I = 1 \) and \( 0.99 \leq \frac{\omega}{\omega_{n,e0}} \leq 1.01 \) ......................................................... 62

Figure 4.11: Spin \( I = 3/2 \) and \( 0.95 \leq \frac{\omega}{\omega_{n,e0}} \leq 1.05 \) ......................................................... 63

Figure 4.12: The Gottfried Angular Velocity \( \left( \frac{\partial \beta}{\partial t} \right) \) vs. Time ............................................. 66

Figure 4.13: The Computational Result for RWA Theory Spin \( I = \frac{1}{2} \) Result .................................. 67

Figure 4.14: The Computational Result for Gottfried Spin \( I = \frac{1}{2} \) Result .................................. 68

Figure 4.15: The Computational Results for the Present RWA Theory for Spin \( I = 1 \) .... 70

Figure 4.16: The Computational Results for Gottfried’s Spin \( I = 1 \) ................................. 71

Figure 4.17: The Computational Result for Spin \( I = 1 \) and \( J = \frac{1}{2} \) Result with \( \omega \) Ranging from 0 to 200000 ......................................................... 77

Figure 4.18: The Computational Result for Spin \( I = 1 \) and \( J = \frac{3}{2} \) Result with \( \omega \) Ranging from 0 to 200000 ......................................................... 80

Figure 4.19: The Computational Result for Spin \( I = 1 \) and \( J = \frac{5}{2} \) Result with \( \omega \) Ranging from 0 to 200000 ......................................................... 84

Figure 4.20: The Computational Result for Spin \( I = \frac{3}{2} \) and \( J = \frac{1}{2} \) Result with \( \omega \) Ranging from 0 to 200000 ......................................................... 87
Figure E.4: The Situation to Considering the Diagonal Terms with 3 Rank 2 Orange Squares for $H_{eff}$ .......................... 162

Figure E.5: The Situation to Considering All Rank 2 Orange Squares for $H_{eff}$ .................. 162

Figure F.1: Spin $I = \frac{5}{2}$ ................................................................. 165

Figure F.2: Spin $I = 3$ ................................................................. 166

Figure F.3: Spin $I = \frac{7}{2}$ ................................................................. 167

Figure F.4: Spin $I = 4$ ................................................................. 168

Figure F.5: Spin $I = \frac{9}{2}$ ................................................................. 169

Figure G.1: Spin $I = 2$ and $0.99 \leq \frac{\omega}{\omega_{n,e}} \leq 1.01$ ................................................................. 172

Figure G.2: Spin $I = \frac{5}{2}$ and $0.99 \leq \frac{\omega}{\omega_{n,e}} \leq 1.01$ ................................................................. 173

Figure G.3: Spin $I = \frac{7}{2}$ and $0.995 \leq \frac{\omega}{\omega_{n,e}} \leq 1.005$ ................................................................. 174

Figure G.4: Spin $I = \frac{7}{2}$ and $0.995 \leq \frac{\omega}{\omega_{n,e}} \leq 1.005$ ................................................................. 175

Figure G.5: Spin $I = 4$ and $0.995 \leq \frac{\omega}{\omega_{n,e}} \leq 1.005$ ................................................................. 176

Figure G.6: Spin $I = \frac{9}{2}$ and $0.995 \leq \frac{\omega}{\omega_{n,e}} \leq 1.005$ ................................................................. 177

Figure I.1: $I=1$ and $J=3/2$ Original Magnetic Dipole and Electric Quadrupole Moment Matrix ................................................................. 181

Figure I.2: The Matrices After First Reduction from the Rank-12 Matrix ......................... 182
LIST OF TABLES

Table 3.1: The Properties of The Stable Isotopes ............................... 39
CHAPTER 1: INTRODUCTION

This chapter provides a comprehensive introduction to the historical development of Nuclear Magnetic Resonance (NMR) along with an elucidation of the terminology and techniques commonly employed in the field of NMR spectroscopy.

Stern-Gerlach Experiment

The original idea of nuclear magnetic resonance started with the Stern-Gerlach experiment. Otto Stern began the concept in 1921, one year after the experiment was successfully run with Walther Gerlach [1]. They used silver atoms shooting past an inhomogeneous magnet field, since the silver atoms have random initial spin direction, based on classical mechanics the silver atoms should formed a continuous vertical line mark on the screen, since the initial silver atoms had random orientations before entering the magnet field and silver atoms had spin $|\frac{1}{2}\rangle$ or $|\frac{-1}{2}\rangle$ (Fig. 1.1 (a)). However, the silver atoms left two distinct marks, one on the top of the screen and one on the bottom of the screen (Fig. 1.1 (b)).
After the Stern-Gerlach experiment, Rabi, Zacharias, Millman, and Kusch proposed a new method to measure nuclear magnetic moments in 1938, and it was the early concept of nuclear magnetic resonance [2]. The concept of early NMR machine would apply a constant magnet field in the $\hat{z}$ (vertical) direction and a weaker magnetic field oscillating in the $\bar{xy}$ (horizontal) plane.

$$B(t) = B_0 \hat{z} + B_1 [\hat{x} \cos(\omega t) + \hat{y} \sin(\omega t)].$$  (Fig. 1.2)
In 1946, Purcell, Torrey, and Pound made a significant contribution to the field with the publication of their paper on resonant absorption in solids, demonstrating that NMR could indeed be observed in solid materials [3]. In the same year, Bloch also published a seminal paper on nuclear induction within an NMR system. This paper elucidates that spin orientation can be achieved not only through a weak oscillatory RF field in the $\bar{x}y$ plane but also via a pulse signal designed to disorient the spin [4]. Later, in 1951, American physicist Russell H. Varian, leveraging his expertise in radio frequency waves, successfully patented the design of the first NMR machine [5].

In the early days, operating NMR machines was challenging, particularly in maintaining a homogeneous $B_0$ field along the vertical direction. This difficulty arose because the sample’s position would slightly vary each time it was installed in the machine. Additionally, due to the unique molecular structures of different samples, the effective $B$ field in the vertical direction could vary between samples.

Modern-day NMR machines integrate many features. For instance, the spinning process, which
was once manual, has been replaced by digital analogs, and the shimming process can now be au-
tomated. NMR technology has evolved into two main types: solution NMR and solid-state NMR
(ssNMR). Solution NMR offers the advantage of high resolution, with samples dissolved in sol-
vents as liquids. However, its application is generally limited to simpler molecules. In contrast,
ssNMR retains the sample in its solid form, enabling the detection of both structure and dynamics
of solid samples. Nevertheless, ssNMR spectra are often more challenging to interpret compared
to solution NMR. The spectra in ssNMR typically lack the distinct, sharp spikes seen in solution
NMR. Despite this, ssNMR is capable of studying molecules that are insoluble in solvents.

Definitions of Terms Relevant to NMR

Chemical Shift ($\delta$): The difference in resonance frequency of a nucleus within a sample relative to
a standard reference frequency. This parameter is pivotal to Nuclear Magnetic Resonance (NMR)
spectroscopy, as it provides insights into the nuclear environment influenced by the molecular
structure and electronic effects surrounding the nucleus. Chemical shifts are quantitatively ex-
pressed in parts per million (ppm), facilitating the precise identification and analysis of molecular
interactions and configurations.

Larmor frequency: The resonance frequency of the NMR, it can be written as $\omega = \gamma B_0$. $\gamma$ is the
gyromagnetic ratio which is the ratio of the magnetic moment to the angular momentum. $B_0$ is the
magnetic field along the $\hat{z}$ axis.

Spin-Spin Coupling ($J$-Coupling): It occurs when the magnetic field generated by the spin of
neighboring nuclei influences the observed nucleus within a molecular structure. This interaction leads to the splitting of the NMR signal of the observed nucleus into multiplets. The coupling constant \( (J) \) quantifies the strength of this interaction, usually measured in Hz.

Decoupling: A technique used to eliminate the effects of \( J \)-Coupling between nuclei, thereby simplifying the NMR spectrum. This simplification facilitates easier interpretation of the spectral data.

\( T_1: \) The spin-lattice relaxation time. It describes the time after the nuclear spin has been knocked off its \( \vec{H}_0 \) direction by the oscillatory field and before it aligns to \( H_0 \) again.

\( T_2: \) The spin-spin relaxation time. It describes how fast the spin with its near spins will lose its coherence due to the interaction with its neighboring spins [4]. \( T_2 \) is the time after the spins knocked off by oscillatory field in the \( \vec{x} \vec{y} \) plane usually until the magnetization decays to 37% of its initial value (the value when the spin was knocked off).
Fig. 1.3 part (a) represents the frontal aspect of the solution-type NMR apparatus, which requires the test sample to be introduced from the top. Part (b) depicts the overhead view of the solution-type NMR instrument, featuring a red ring-shaped compartment specifically designated for the insertion of test samples. Part (c) shows the solution NMR test sample along with its holder and measurement tool, designed to ensure the correct positioning of the test sample when inserted through the red top entrance in part (b).
Fig. 1.4 illustrates the solid-state NMR (ssNMR) system in detail. Part (a) showcases the frontal view of the ssNMR apparatus, where samples are inserted from the bottom. Part (b) displays the rotor, which contains the sample, along with the rotor cap. Part (c) depicts the mechanism that assists in the installation of the rotor into the probe. Part (d) is the probe, designed for the insertion of the rotor with the sample. This probe is inserted into the ssNMR apparatus from its base.
The Relevant Techniques in NMR

*Multiple-Pulse Sequences*

Before the multiple pulse sequences, let’s talk about a basic pulse sequence.

![Figure 1.5: A Basic Pulse Sequence](image)

**Fig. 1.5** is a basic pulse sequence $f(t)$. Part (a) is the relaxation decay of the electromagnetic induction, also known as Free Induction Decay (FID). Part (b) is the Fourier transform $F(\omega)$ of the FID graph. The Fourier transform of a pulse $f(t)$ is given by

$$F(\omega) = \int_{-\infty}^{\infty} f(t) e^{-i\omega t} dt \quad (1.1)$$

Equation (1.1) is for Fourier transforming the raw NMR $f(t)$ data of free induction decay to processed NMR data with spikes. For a basic pulse sequence, the process representing figure 1.5
from part (a) to part (b). The inverse transform of \( F(\omega) \) is given by

\[
f(t) = \int_{-\infty}^{\infty} F(\omega) e^{i\omega t} d\omega \quad (1.2)
\]

Similarly, Eqn. 1.2 is for transforming the processed NMR data back to the raw NMR data of free induction decay. For a basic pulse sequence, the process representing Fig. 1.5 from part (b) to part (a).

A multiple pulse sequence can excite different atomic nuclei, since different nuclei have different resonance frequencies. The multiple pulse sequence can excite one type of nuclei first, then the nuclei can also create a buffer for exciting the other types of nuclei. The purposes of multiple pulse sequences include enhance resolution, filtering information, and 2 dimensional (2D) NMR. For example, for a complex organic sample which contains \(^1\)H and \(^{13}\)C, one can use the Heteronuclear Single Quantum Coherence (HSQC) 2D technique[6] to spread the peaks on a 2D plane to identify the molecule structure, chemical shift, and to enhance the resolution of the spectrum.

Dilution

Dilution is a process in chemistry that involves reducing the concentration of solutes by increasing the amount of solvent or decreasing the solute amount. Sometimes, a highly concentrated testing sample may present problems with overlapping resonance peaks; lowering the concentration can significantly improve the signal clarity. Additionally, in some cases, an overly concentrated sample could lead to peak broadening; thus, diluting the sample can also enhance the signal quality. Furthermore, diluting the sample can reduce intermolecular interactions. For instance, dipole-dipole bonding in a sample can be minimized, thereby ensuring that intermolecular interactions do not alter the chemical shift. Dilution is commonly used in solution NMR.
Magic-Angle Spinning

Magic-angle spinning is a technique to improve the resolution of ssNMR spectra. The standard NMR technique has the weaker oscillating magnetic field perpendicular to the $\hat{z}$ axis and within the $\bar{xy}$ plane. However, the magic angle spinning has the weaker field oscillating with some angle $\theta_m$ with respect to the $\hat{z}$ axis [7].

![Diagram of Magic Angle Spinning Setting](image)

**Figure 1.6: The Magic Angle Spinning Setting**

For states $|I, m_I\rangle$ and $|S, m_s\rangle$, ...
\[ I_z |I, m_I\rangle = \hbar m_I |I, m_I\rangle \]
\[ I_x = \frac{1}{2} (I^+ + I^-) \]
\[ I_y = \frac{1}{2i} (I^+ - I^-) \]
\[ I_\pm |I, m_I\rangle = \hbar \sqrt{I(I+1) - m_I (m_I \pm 1)} |I, m_I \pm 1\rangle \]

Where \( I_{pm} = I_x \pm i I_y \), and similarly for \( S_z, S_x, S_y, \) and \( S_\pm \).

The Hamiltonian for magnetic dipolar interactions between two adjacent spins \( I \) and \( S \) can be written as [8]:
\[ H_D = \frac{\hbar^2 \gamma_I \gamma_S}{r^3} \left[ I \cdot S - 3 \frac{(I \cdot r)(S \cdot r)}{r^2} \right] \]
\[ = \frac{\hbar^2 \gamma_I \gamma_S}{r^3} [A + B + C + D + E + F] \]

Where
\[ A = I_z S_z (1 - 3 \cos^2 \theta) \]
\[ B = -\frac{1}{4} \left( 1 - 3 \cos^2 \theta \right) (I^+ S^- + I^- S^+) \]
\[ C = \frac{3}{2} \sin \theta \cos \theta e^{-i\varphi} (I_z S^+ + S_z I^+) \]
\[ D = C^\dagger \]
\[ E = \frac{3}{4} \sin^2 \theta I^+ S^+ e^{-2i\varphi} \]
\[ F = E^\dagger \]

and \( r \) is the vector of displacement from \( I \) to \( S \), \( r \) is the distance, \( \theta \) is the polar angle along the vertical direction, and \( \varphi \) is the azimuthal angle along the horizontal direction. Magic angle spinning happen when \( 1 - 3 \cos^2 \theta = 0 \) and \( \theta = 54.75^\circ \).

Magic Angle spinning can effectively reduce the nuclear spin dipole interactions within the solid state sample to make the broaden of spectra narrow [9]. The magic angle spinning effect is shown below.
Cross polarization

Cross polarization is an enhanced intensity technique mostly used in ssNMR. For example, for an amino acid sample, the polarization of the common $^1\text{H}$ can be transferred to $^{15}\text{N}$ which has lower abundance. Therefore the process can enhance the signal intensity of $^{15}\text{N}$ and reduce the experiment time.
CHAPTER 2: LITERATURE REVIEW

The exploration of NMR state probabilities commenced with Güttinger’s 1931 paper, introducing the concept of a rotating magnetic field [10]. Subsequently, Majorana published his findings in 1932, presenting the probabilities for transition between single states without offering derivations [11]. In 1937, Schwinger identified and addressed issues in Güttinger’s approach, proposing a solution [12]. However, Schwinger’s unconventional method led to its underrecognition. The integration of theoretical and experimental perspectives was achieved in a 1954 publication by Rabi, Ramsey, and Schwinger, which outlined the probabilities of state functions incorporating $T_1$ and $T_2$ [13]. Gottfried’s 1966 book further evolved NMR theory by introducing a novel calculation method for the probabilities of transitions between individual states [14]. Modern NMR theory primarily builds upon Gottfried’s probability function, despite challenges in calculating mixed states and accounting for initial phase shifts.

Güttinger, 1931

In 1931, Güttinger introduced rotational frame in his paper for solving NMR problems [10]. Güttinger thought the inhomogeneous system of the magnetic field in the Stern-Gerlach experiment can be used as an inhomogeneous time system for NMR. Güttinger used the standard perturbation theory try to solve the NMR problem, but he made his assumptions of knowing each individual energy level $E_m(t)$ for state $m$ at the time $t$. The general procedure was rotate the reference frame along a certain axis. In the NMR system, Güttinger suggested to rotate the reference frame anticlockwise about the $\hat{z}$ axis. As an example, he wrote a general solution for spin $J = \frac{1}{2}$ case.
\[ \psi = C^{-1/2}u^{-1/2} + C^{+1/2}u^{+1/2} \]
\[ C^{-1/2} = \varrho^{-1/2} \left( -\cos \frac{\Theta}{2} \right) e^{-\pi it\sqrt{(og)^2 + v^2}} + \varrho^{+1/2} \left( \sin \frac{\Theta}{2} \right) e^{\pi it\sqrt{(og)^2 + v^2}} \]
\[ C^{+1/2} = \varrho^{-1/2} \left( \sin \frac{\Theta}{2} \right) e^{-\pi it\sqrt{(og)^2 + v^2}} + \varrho^{+1/2} \left( \cos \frac{\Theta}{2} \right) e^{\pi it\sqrt{(og)^2 + v^2}} \]

where \( o \) is the larmor frequency, \( g \) is the landé g-factor, and \( \upsilon \) is the rotation frequency.

And if \( t = 0 \), \( C^{-1/2} = 0 \), and \( C^{+1/2} = 1 \) then the equation (2.1) reduced to,

\[ C^{-1/2} = \varrho^{-1/2} \left( -\cos \frac{\Theta}{2} \right) + \varrho^{+1/2} \left( \sin \frac{\Theta}{2} \right) = 0 \]  
\[ C^{+1/2} = \varrho^{-1/2} \left( \sin \frac{\Theta}{2} \right) + \varrho^{+1/2} \left( \cos \frac{\Theta}{2} \right) = 1 \]  

Therefore, it is established, that

\[ \varrho^{-1/2} = \sin \frac{\Theta}{2} \]  
\[ \varrho^{+1/2} = \cos \frac{\Theta}{2} \]  

Where \( \tan \Theta = \frac{\upsilon}{og} \).

The probability of \( m = -1/2 \) can be written as:

\[ |C^{-1/2}|^2 = \frac{\upsilon^2}{(og)^2 + \upsilon^2} \sin^2 \left( \pi t \sqrt{(og)^2 + \upsilon^2} \right) \]  

and the probability of \( m = 1/2 \) can be written as

\[ |C^{+1/2}|^2 = \left| \cos \left( \pi t \sqrt{(og)^2 + \upsilon^2} \right) + i \frac{og}{\sqrt{\upsilon^2 + (og)^2}} \sin \left( \pi t \sqrt{(og)^2 + \upsilon^2} \right) \right|^2 \]  

The problem with Güttinger’s rotational frame is that his calculation did not consider the rotational frame factor inside the \( \sqrt{(og)^2 + \upsilon^2} \) term. And the way of rotation also cannot show the resonance frequency of the NMR.
For the transition probabilities from each of the $m$ states to $m'$ states, Güttinger listed a complex polynomial system for the calculation

$$J_0(p, q; u) = 1,$$

$$J_1(p, q; u) = q - (p + 1) u$$

$$J_2(p, q; u) = q (q + 1) - 2 (q + 1) (p + 2) u + (p + 2) (p + 3) u^2$$

$$J_n (p, q; x) = q (q + 1) \cdots (q + n - 1) \cdot F(p + u, -n, q; x)$$

and,

$$F(\alpha, \beta, \gamma; x) = (1 - x)^{\gamma - \alpha - \beta} F(\gamma - \beta, \gamma - \alpha, \gamma; x)$$

$$= (1 - x)^{-\alpha} F(\alpha, \gamma - \beta, \gamma; \frac{x}{x - 1})$$

$$= (1 - x)^{\beta} F(\beta, \gamma - \alpha, \gamma; \frac{x}{x - 1})$$

The general transition equation

$$S_{m,m'} = \sqrt{\frac{\binom{2j}{j-m}}{\binom{2j}{j-m'}}} e^{i(m'\Psi + m\psi) + \frac{ij}{2}(m + m')} \cdot \left(\sin \frac{\Theta}{2}\right)^{m'-m} \cdot \left(\cos \frac{\Theta}{2}\right)^{m + m'}$$

$$\times J_{j-m'} \left(2m' + 1, m + m' + 1; \cos^2 \frac{\Theta}{2}\right)$$

$$= \sqrt{\frac{\binom{2j}{j-m}}{\binom{2j}{j-m'}}} \sum_{(p)} \left(\cos \frac{\Theta}{2}\right)^{2p-m-m'} \left(i \sin \frac{\Theta}{2}\right)^{2j+m+m'-2p} \binom{j+m}{p} \binom{j-m}{j+m'-p}$$

where $\tan \Theta = \frac{v}{ogy}$, and $\psi, \Psi$ are the corresponding functions for $m$ and $m'$ states. Güttinger’s polynomial system is a very complex summation for doing the calculation. Based on Güttinger’s system, it is essential to determine the distribution of each spin $m$ state initially at $t = 0$, without any initial phase shift. Subsequently, the transition matrix and the probability distribution across all spin states can be calculated.
In 1932, Majorana published his paper that identified the problem with Güttinger’s formula related to the calculation of a non-adiabatic transition [11]. Majorana listed his own formula

\[ W(P, P'; m, m') = \left( \cos \frac{\alpha}{2} \right)^{4j} \frac{(j + m)! (j - m)! (j + m')! (j - m')!}{\sum_{r=0}^{\infty} \frac{(-1)^r (\tan \frac{\alpha}{2})^{2r-m+m'} r! (r - m + m')! (j + m - r)! (j - m' - r)!}{r! (r - m + m')! (j + m - r)! (j - m' - r)!}} \]  

(2.9)

However, the Majorana formula did not consider the potential initial phase factor and only can work for cases of a single state transforming to another single state. Majorana stated that the spin \( J > \frac{1}{2} \) systems can be treated as multiple spin \( \frac{1}{2} \) systems combined. But the derivation from the spin \( J = 1/2 \) system to spin \( J > 1/2 \) systems was left out of Majorana’s paper. In his paper, Majorana listed the solution of transition probability from state \( m = -\frac{1}{2} \) to state \( m' = \frac{1}{2} \).

\[ W\left(-\frac{1}{2}, \frac{1}{2}\right) = \sin^2 \frac{\alpha}{2} \]  

(2.10)

where \( \alpha = 2 \arcsin e^{-\frac{kx}{\bar{\hbar}}} \).

By assuming at an instant of the general form for nuclear spin, \( H_x = A, H_y = 0, \) and \( H_z = -Ct \).

\[ k = \frac{g\mu_0 A^2}{\bar{\hbar}C} \]

Schwinger, 1937

In 1937 Schwinger addressed the generalized Güttinger equation [12],

\[ i\hbar \frac{\partial C_m}{\partial t} - E_mC_m = i\hbar \sum_{m' \neq m} \frac{\langle m | \partial H / \partial t | m' \rangle}{E_m - E_{m'}} C_{m'} - i\hbar \left( \Psi_m, \frac{\partial \Psi}{\partial t} \right) C_{m'} \]  

(2.11)
which he was unable to solve without knowing, \( \mathcal{H}(t) \Psi_m(t) = E_m(t) \Psi_m(t) \).

For the Hamiltonian:

\[
\mathcal{H}(t) = -g\mu_0 \mathbf{J} \cdot \mathbf{H}(t)
\]

and the magnetic field

\[
\mathbf{H}(t) = H (i \sin \vartheta \cos \gamma + j \sin \vartheta \sin \gamma + k \cos \vartheta)
\]

Where, \( H, \vartheta, \) and \( \gamma \) are functions of time. Then, Schwinger refocused on \( \mathcal{H}(t) \Psi_m(t) = E_m(t) \Psi_m(t) \) and rewrote the state function into the form

\[
\Phi = e^{iJ_y \vartheta} \sum_m C'_m \Psi_m^{(0)} e^{-(i\hbar E_m')t}
\]

where

\[
E_m' = -m' \frac{\hbar \omega \sin \vartheta}{\sin \Theta}, \quad \tan \Theta = \frac{\hbar \omega \sin \vartheta}{\hbar \omega \cos \vartheta + g\mu_0 H}
\]

by using the rotational relations between \( J_x, J_y, \) and \( J_z, \)

\[
e^{iJ_x \psi} J_x e^{-iJ_x \psi} = J_x \cos \psi - J_y \sin \psi \\
e^{iJ_x \psi} J_y e^{-iJ_x \psi} = J_x \sin \psi + J_y \cos \psi \\
e^{iJ_y \vartheta} J_x e^{-iJ_y \vartheta} = \cos \vartheta J_x + \sin \vartheta J_z \\
e^{iJ_y \vartheta} J_z e^{-iJ_y \vartheta} = -\sin \vartheta J_x + \cos \vartheta J_z.
\]

In here, Schwinger’s rotations are anti-clockwise. In chapter 3 section 3.1, the similar procedures are clockwise. Schwinger found
\[ C_m(t) = \sum_{m'} \langle m | e^{iJ_y \Theta} | m' \rangle \langle m' | e^{(i/h)\gamma t J_z} | m'' \rangle \langle m'' | e^{-iJ_y \Theta} | m''' \rangle C_{m'''}(0) \]

\[ = \sum_{m'} \langle m | e^{iJ_y \Theta} e^{(i/h)\gamma t J_z} e^{-iJ_y \Theta} | m' \rangle C_{m'}(0) \quad (2.17) \]

where \( \gamma = \sqrt{g^2 \mu_0^2 H^2 + 2g \mu_0 H \hbar \omega \cos \vartheta + \hbar^2 \omega^2} \). The solution, which closely resembles Eqn. (3.44) in chapter 3, was obtained by employing the rotation field method. However, the primary difference between Schwinger’s Eqn. (2.17) and Eqn. (3.44) lies in the direction of the rotation. Specifically, Schwinger’s Eqn. (2.17) cannot determine the Larmor frequency due to the rotation’s direction.

The transition probabilities \( W \) from an initial state \( m \) to a later state \( m' \) at time \( t \) by using

\[ W(m, m'; t) = \left| \langle m' | e^{iJ_y \Theta} e^{(i/h)\gamma t J_z} e^{-iJ_y \Theta} | m \rangle \right|^2 \]

\[ = \left| \langle m' | e^{(i/h)\gamma t (J_z \cos \Theta - J_x \sin \Theta)} | m \rangle \right|^2 \quad (2.18) \]

Finally, Schwinger compared the transition from \( m = 1/2 \) to \( m = -1/2 \) for spin \( \frac{1}{2} \) case in both the Güttinger solution and the Schwinger solution,

Güttinger solution:

\[ W \left( \frac{1}{2}, -\frac{1}{2}; t \right) = \frac{\hbar^2 \omega^2 \sin^2 \vartheta}{g^2 \mu_0^2 H^2 + \hbar^2 \omega^2 \sin^2 \vartheta} \frac{t}{2\hbar} \]

\[ \times \left( g^2 \mu_0^2 H^2 + \hbar^2 \omega^2 \sin^2 \vartheta \right)^\frac{1}{2} \quad (2.19) \]

Schwinger solution:

\[ W \left( \frac{1}{2}, -\frac{1}{2}; t \right) = \frac{\hbar^2 \omega^2 \sin^2 \vartheta}{g^2 \mu_0^2 H^2 + 2g \mu_0 H \hbar \omega \cos \vartheta + \hbar^2 \omega^2 \sin^2 \vartheta} \frac{t}{2\hbar} \]

\[ \times \left( g^2 \mu_0^2 H^2 + 2g \mu_0 H \hbar \omega \cos \vartheta + \hbar^2 \omega^2 \sin^2 \vartheta \right)^\frac{1}{2} \quad (2.20) \]

Schwinger correctly addressed the issue with Güttinger equation, and correctly listed the probabilities of transitions from one state to another state cases. However, Schwinger’s equation rotated the field in the opposite direction, which was outside the range of the resonance frequency.
In 1954, Rabi, Ramsey, and Schwinger used the rotational coordinate system to solve the problem \[13\]. They used $H_1$ as the rotating magnetic field in the $\bar{x}y$ plane, and $H_0$ as the perpendicular constant magnetic field along the $\hat{z}$ axis. Next, they rotated the coordinate system along the $\hat{z}$ axis with frequency $-\omega$. They identified that only clockwise rotations could find the resonance, which was different from Schwinger’s paper in 1937\[12\]. So that for $H_0 = H_0 \mathbf{k}$, $H_1 = H_1 \mathbf{i}$, and $\omega = -\omega$, they found $H_{er} = (H_0 - \omega/\gamma) \mathbf{k} + H_1 \mathbf{i}$. Where, $|H_{er}| = [(H_0 - \omega/\gamma)^2 + H_1^2]^{\frac{1}{2}} = a/\gamma$ and $\gamma$ is the gyromagnetic ratio. Then they also used a classical interpretation of the nuclear resonance experiments. For a time interval $t_2 - t_1$,

$$P_{+\frac{1}{2}} = \frac{1 - \cos \alpha}{2} = \sin^2 \Theta \sin^2 \frac{a(t_2 - t_1)}{2} = \left(\frac{\omega_0 H_1/H_0}{(\omega_0 - \omega)^2 + \omega_0 H_1/H_0^2}\right) \sin^2 \frac{a(t_2 - t_1)}{2} \quad (2.21)$$

In here, angle $\alpha$ is for the angle between constant field $\mathbf{H}_0$ in the $\hat{z}$ direction and the particle spin $\mathbf{I}_z$’s direction. Initially, $\mathbf{H}_0$ and $\mathbf{I}$ have the aligned to each other, before the oscillatory field within the horizontal plane (the $\bar{x}y$ plane) is introduced into the system.

$$P_{+\frac{1}{2}} + P_{-\frac{1}{2}} = 1 \quad (2.22)$$

They also showed an approximation for the average net absorption rate $R$ of energy

$$R = W n_s \hbar \omega = (1/8) \gamma^2 H_1^2 T_2 N \hbar^2 \omega^2 / k_B T, \quad (2.23)$$
where $N$ is the number of nuclei, and $T$ is the temperature. $n_s = \frac{1}{2} N \hbar \omega / k_B T$ is the rest nuclei in lowest energy state, $T_2$ is the characteristic time for the spins to lose coherence with their neighbors.

At the end, Rabi, Ramsey, and Schwinger showed that the probability of a transformation from the $m$ state to the $m'$ state can be written as

$$P_{m' \leftarrow m} = |\langle m' | \exp (i \omega t_2 k \cdot \mathbf{I}) \exp (-i \omega t_1 k \cdot \mathbf{I}) | m \rangle|^2$$

$= |\langle m' | \exp (i a [t_2 - t_1] \alpha \cdot \mathbf{I}) | m \rangle|^2$,

(2.24)

where $\alpha$ is the unit vector parallel to $H_{er}$, and $H_{er}$ is the total effective magnetic field. However, the transition from the $m$ state to the $m'$ state was not fully diagonalized.

Gottfried, 1966

In Gottfried’s book [14], he used the Heisenberg picture $J(t) = e^{-i \Omega t J_z / \hbar} J e^{i \Omega t J_z / \hbar}$ to rotate the magnetic field along the $\hat{z}$ axis, where $\Omega$ is the Larmor frequency. The state function for can be written as

$$|t\rangle_R = e^{i \omega t J_z / \hbar} e^{-i (\omega - \Omega) J_z - \lambda \Omega J_x t / \hbar} |0\rangle$$

(2.25)

where $\lambda << 1$, since the magnetic field along the $\hat{z}$ axis is much stronger than the oscillating magnetic field.

Gottfried also gave his general formula for the probability from one $m$ state to another $m'$ state.

$$p_j (m'm; t) = |d^{(j)}_{m'm}(\beta)|^2$$

(2.26)

where $\beta$ is the second Euler angle, determined by $\sin \frac{\beta}{2} = (\lambda \Omega / \Delta) \sin \frac{\Delta t}{2}$. And $\Delta^2 = (\omega - \Omega)^2 + (\lambda \Omega)^2$. 

20
Gottfried also gave an example for the spin $\frac{1}{2}$ case,

$$p_{\frac{1}{2}} (m' \neq m; t) = \left( \frac{\lambda \Omega}{\Omega - \omega} \right)^2 \sin^2 \left( \frac{(\Omega - \omega) t}{2} \right)$$ \hspace{1cm} (2.27)

At the resonance frequency $\omega = \Omega$, the Eqn. 2.27 becomes,

$$p_{\frac{1}{2}} (m' \neq m; t) = \frac{1}{4} (\lambda \Omega t)^2$$ \hspace{1cm} (2.28)

Gottfried’s example for spin $\frac{1}{2}$ case accurately described the probabilities of each spin state. However, the general spin state in Eqn.(2.26) only partially correct. The Eqn. (2.26) only works for the cases of the probabilities of one single state $m$ transforming to another single state $m'$, but Eqn. (2.26) is unable to accurately predict the probabilities from one mixed state to another mixed state. For example, the Eqn. (2.26) cannot predict any entangled state cases. In addition, the Gottfried’s formula depends on the Euler rotational angle $\beta(t)$ from $\sin \frac{\beta}{2} = (\lambda \Omega / \Delta) \sin \frac{\Delta t}{2}$, and $\beta(t)$ is not a fixed angle or a rotation with a constant angular velocity. Therefore, the Gottfried’s equation is not sufficient to present the full features of any spin case, even for $1/2$ spin.
CHAPTER 3: METHODOLOGY

The Rotating Wave Transformation

In standard NMR, the magnetic field configuration comprises a constant, strong $H_0$ field oriented in the vertical direction, accompanied by a weak, oscillatory $H_1$ field in the horizontal ($\bar{xy}$) plane.

$$H(t) = H_0 \hat{z} + H_1 [\hat{x} \cos(\omega t) + \hat{y} \sin(\omega t)] \quad (3.1)$$

Given that $\dot{H} = \mu_n H(t) \cdot I$, where $\mu_n$ is the nuclear moment. The Hamiltonian for standard NMR is thereby formulated as follows:

$$\dot{H} = \omega_{n0} I_z + \omega_{n1} [I_x \cos(\omega t) + I_y \sin(\omega t)] \quad (3.2)$$

Common nuclear magnetic dipole moment spin quantum numbers $I$ for light stable isotopes include: $I = \frac{1}{2}$ for $^1$H and $^{13}$C; $I = 1$ for $^2$H and $^{14}$N; $I = \frac{3}{2}$ for $^7$Li, $^9$Be, and $^{11}$B; $I = \frac{5}{2}$ for $^{17}$O; $I = 3$ for $^{10}$B; and values extending up to $I = \frac{9}{2}$ for $^{83}$Kr, $^{87}$Sr, $^{93}$Nb, $^{113}$In, $^{179}$Hf, and $^{209}$Bi, with even higher values observed for long-lived unstable nuclei [15, 16]. These quantum numbers play a pivotal role in the foundational theories and experimental practices of standard magnetic resonance [11, 13, 17–19].

The oscillatory magnetic field in the $\bar{xy}$ plane possesses an angular frequency $\omega_{n1}$. It is defined that $\omega_{n0} = \mu_n (1 - \sigma)H_0$, and $\omega_{n1} = \mu_n (1 - \sigma')H_1$. Here, $\sigma$ signifies the chemical shift along the $\hat{z}$
axis corresponding to the magnetic field $H_0$, while $\sigma'$ represents the chemical shift in the direction of the rotating magnetic field $H_1$. Typically, the magnitude of the ratio $|\omega_n/\omega_{n0}| << 1$, indicating the oscillatory field’s frequency is substantially lower than the static field’s frequency. Chemical shifts, representing minor perturbations, are quantified in parts per million (ppm) to reflect the electronic environment surrounding nuclei [11, 13, 14, 17–21]. This metric is crucial in organic chemistry for determining the molecular locations of the nuclei probed [22–24].

The initial wave function may be defined as

$$|\psi(0)\rangle = \sum_{m=-I}^{I} a_m(0) |I, m\rangle.$$  \hspace{1cm} (3.3)

Since the initial state function is normalized, therefore

$$\sum_{m=-I}^{I} |a_m(0)|^2 = 1$$  \hspace{1cm} (3.4)

where the $a_m(0)$ represent the general initial state. The components of the nuclear spin follow the relations,

$$[I_i, I_j] = i\hbar \epsilon_{ijk} I_k,$$  \hspace{1cm} (3.5)

where $\hbar = \frac{\hbar}{2\pi}$, $\hbar$ is Planck’s constant, and $\epsilon_{ijk}$ is the Levi-Civita symbol. For example, $\epsilon_{xyz} = 1$ and $\epsilon_{xzy} = -1$.

The $B_1$ field is oscillating within the $xy$ plane with a constant velocity $\omega$. Therefore, assuming $\phi$ to be the rotational angle of the induced magnetic field within the $xy$ plane, for which $\phi = \omega t$ [21].

$$I_x(\phi) = e^{iI_x\phi/\hbar} I_x e^{-iI_x\phi/\hbar}$$

$$I_y(\phi) = e^{iI_y\phi/\hbar} I_y e^{-iI_y\phi/\hbar}$$  \hspace{1cm} (3.6)

Taking the partial derivative of $I_x$ respect of $\phi$ can finds,
\[
\frac{\partial I_x}{\partial \phi} = \frac{i}{\hbar} e^{iI_z \phi/\hbar} [I_z, I_x] e^{-iI_z \phi/\hbar} = -I_y (\phi), \quad (3.7)
\]

\[
\frac{\partial^2 I_x (\phi)}{\partial \phi^2} + I_x (\phi) = 0. \quad (3.8)
\]

Similarly, taking the partial derivative of \(I_y\) with respect to \(\phi\) can find,

\[
\frac{\partial I_y}{\partial \phi} = \frac{i}{\hbar} e^{iI_z \phi/\hbar} [I_z, I_y] e^{-iI_z \phi/\hbar} = I_x (\phi), \quad (3.9)
\]

\[
\frac{\partial^2 I_y (\phi)}{\partial \phi^2} + I_y (\phi) = 0. \quad (3.10)
\]

The solutions for Eqn. 3.8 and Eqn. 3.10 are in the form.

\[
I_x (\phi) = A \cos (\phi) + B \sin (\phi),
\]

\[
I_y (\phi) = C \cos (\phi) + D \sin (\phi), \quad (3.11)
\]

\(A, B, C, D\) are operators and \(\phi\) is a real constant.

Therefore, after including the initial conditions at \(\phi = 0\) can find,

\[
I_x (\phi) = I_x \cos (\phi) - I_y \sin (\phi)
\]

\[
I_y (\phi) = I_y \cos (\phi) + I_x \sin (\phi) \quad (3.12)
\]

Assume the constant rotation within the \(xy\) plane is negative or clockwise \([14]\), then

\[
I_x (-\omega t) = I_x \cos (\omega t) + I_y \sin (\omega t) = e^{-iI_z \omega t/\hbar} I_x e^{iI_z \omega t/\hbar} \quad (3.13)
\]
Therefore, the Hamiltonian can be written as

\[
\hat{H} = \omega_{n0} I_z + e^{-iI_z \omega t / \hbar} \omega_{n1} I_x e^{iI_z \omega t / \hbar}
\]

\[
= e^{-iI_z \omega t / \hbar} (\omega_{n0} I_z + \omega_{n1} I_x) e^{iI_z \omega t / \hbar}
\]  

(3.14)

Assume \(|\psi\rangle = e^{-iI_z \omega t / \hbar} |\psi'\rangle\), then

\[
i\hbar \frac{\partial |\psi\rangle}{\partial t} = \omega I_z e^{-iI_z \omega t / \hbar} |\psi'\rangle + i\hbar e^{-iI_z \omega t / \hbar} \frac{\partial |\psi'\rangle}{\partial t},
\]

(3.15)

From the Schrödinger equation \(\hat{H} |\psi\rangle = i\hbar \frac{\partial |\psi\rangle}{\partial t}\), the Eqn. (3.15) can be rewritten as

\[
\hat{H} |\psi\rangle = \hat{H} e^{-iI_z \omega t / \hbar} |\psi'\rangle,
\]

\[
e^{-iI_z \omega t / \hbar} (\omega_{n0} I_z + \omega_{n1} I_x) |\psi'\rangle = e^{-iI_z \omega t / \hbar} \left( \omega I_z |\psi'\rangle + i\hbar \frac{\partial |\psi'\rangle}{\partial t} \right),
\]

(3.16)

\[
e^{-iI_z \omega t / \hbar} [ (\omega_{n0} - \omega) I_z + \omega_{n1} I_x ] |\psi'\rangle = i\hbar e^{-iI_z \omega t / \hbar} \frac{\partial |\psi'\rangle}{\partial t}.
\]

Multiplying both sides by equation \(e^{iI_z \omega t / \hbar}\), then

\[
[ (\omega_{n0} - \omega) I_z + \omega_{n1} I_x ] |\psi'\rangle = i\hbar \frac{\partial |\psi'\rangle}{\partial t}.
\]

(3.17)

Therefore, the effective Hamiltonian \(\hat{H}_{eff} = (\omega_{n0} - \omega) I_z + \omega_{n1} I_x\) is independent of the time \(t\). Therefore, the vectors can be normalized as.

\[
\hat{u}_z = \hat{z} \frac{\omega_{n0} - \omega}{\Omega}
\]

\[
\hat{u}_x = \hat{x} \frac{\omega_{n1}}{\Omega}
\]

(3.18)

Where \(\Omega = \sqrt{(\omega_{n0} - \omega)^2 + \omega_{n1}^2}\), and \(\hat{u} \cdot \hat{u} = 1\).
At the last, the Schrödinger equation can be rewritten as:

$$\hat{H}_{\text{eff}} |\psi'\rangle = [(\omega_{n0} - \omega) I_z + \omega_{n1} I_x] |\psi'\rangle = i\hbar \frac{\partial |\psi'\rangle}{\partial t}$$

(3.19)

Diagonalize the Effective Hamiltonian

The method employed for diagonalizing the effective Hamiltonian is analogous to the technique used in solving a Rubik’s cube, involving a strategic rotation approach.

![Image](image.png)

Figure 3.1: The Process of Fixing a Rubik’s Cube

Consider $\hat{H}_{\text{eff}} = [(\omega_{n0} - \omega) I_z + \omega_{n1} I_x]$ where the term $\omega_{n1} I_x$ is analogous to an undesired square within a row on a Rubik’s cube, which necessitates a rotation out of the row. This concept can be likened to the extra portion from the diagonalized part being rotated out. The procedure is illustrated from part (a) to part (b), and from part (c) to part (d) in Fig. 3.1.
\[ e^{-i\beta n I_y/\hbar} H_{\text{diag}} e^{i\beta n I_y/\hbar} = H_{\text{eff}} = (\omega_n - \omega) I_z + \omega_n I_x \] (3.20)

The next step is to find the rotational angle and the axis which can perform the rotation.

\[ H_{\text{diag}} = e^{i\beta n I_y/\hbar} H_{\text{eff}} e^{-i\beta n I_y/\hbar} = (\omega_n - \omega) e^{i\beta n I_y/\hbar} I_z e^{-i\beta n I_y/\hbar} + \omega_n e^{i\beta n I_y/\hbar} I_x e^{-i\beta n I_y/\hbar} \] (3.21)

Assuming, \( I_z (\beta_n) = e^{i\beta n I_y/\hbar} I_x e^{-i\beta n I_y/\hbar} \) and \( I_x (\beta_n) = e^{i\beta n I_y/\hbar} I_x e^{-i\beta n I_y/\hbar} \).

Therefore,

\[ \frac{\partial I_z (\beta_n)}{\partial \beta_n} = e^{i\beta n I_y/\hbar} [I_y, I_z] e^{-i\beta n I_y/\hbar} \]

\[ = - I_x (\beta_n) \] (3.22)

Similarly,

\[ \frac{\partial I_x (\beta_n)}{\partial \beta_n} = e^{i\beta n I_y/\hbar} [I_y, I_x] e^{-i\beta n I_y/\hbar} \]

\[ = I_z (\beta_n) \] (3.23)

Taking the partial derivative of these equations with respect of angle \( \beta \) again and arrange the terms can find:

\[ \frac{\partial^2 I_z (\beta_n)}{\partial \beta_n^2} + I_z (\beta_n) = 0 \] (3.24)

\[ \frac{\partial^2 I_x (\beta_n)}{\partial \beta_n^2} + I_x (\beta_n) = 0 \] (3.25)

After including the boundary conditions \( (I_z (0) = I_z, I_x (0) = I_x, I_z' (0) = -I_x (0), I_x' (0) = I_z (0)) \) into the general solutions, the solutions become:

\[ I_z (\beta_n) = I_z \cos (\beta_n) - I_x \sin (\beta_n) \]

\[ I_x (\beta_n) = I_x \cos (\beta_n) + I_z \sin (\beta_n) \] (3.26)

Now, \( H_{\text{diag}} \) can be written as

27
\[ H_{\text{diag}} (\beta_n) = (\omega_{n0} - \omega) I_z (\beta_n) + \omega_{n1} I_x (\beta_n) \]
\[ = (\omega_{n0} - \omega) [I_z \cos (\beta_n) - I_x \sin (\beta_n)] + \omega_{n1} [I_x \cos (\beta_n) + I_z \sin (\beta_n)] \]
\[ = [(\omega_{n0} - \omega) \cos (\beta_n) + \omega_{n1} \sin (\beta_n)] I_z + [-(\omega_{n0} - \omega) \sin (\beta_n) + \omega_{n1} \cos (\beta_n)] I_x \]
\[ (3.27) \]

Since \( H_{\text{diag}} \) should only contain the diagonal terms, the \( I_x \) term has to be forced equal to zero.

\[ - (\omega_{n0} - \omega) \sin (\beta_n) + \omega_{n1} \cos (\beta_n) = 0, \]
\[ \tan (\beta_n) = \frac{\sin (\beta_n)}{\cos (\beta_n)} = \frac{\omega_{n1}}{\omega_{n0} - \omega}, \]
\[ (3.28) \]

Therefore,
\[ \sin (\beta_n) = \frac{\omega_{n1}}{\Omega_n}, \]
\[ \cos (\beta_n) = \frac{\omega_{n0} - \omega}{\Omega_n}, \]
\[ (3.29) \]

and,
\[ \Omega_n = \sqrt{(\omega_{n0} - \omega)^2 + \omega_{n1}^2}. \]
\[ (3.30) \]

The functions \( \tan (\beta_n), \sin (\beta_n), \) and \( \cos (\beta_n) \) are all applicable for determining the angle \( \beta_n \).

However, given that \( \tan (\beta_n) \) may approach infinity under certain conditions, the calculation of the angle \( \beta_n \) typically relies on the \( \sin (\beta_n) \) or \( \cos (\beta_n) \) functions as specified in Eqn. (3.29).

\[ \hat{H}_{\text{diag}} = \Omega_n I_z \]
\[ \hat{H}_{\text{eff}} = e^{-i\beta_n I_y/\hbar} \Omega_n I_z e^{i\beta_n I_y/\hbar} \]
\[ (3.31) \]

where \( \beta_n = \sin^{-1} \left( \frac{\omega_{n1}}{\Omega_n} \right) \).

The variance between the Hamiltonians \( \hat{H}_{\text{eff}} \) and \( \hat{H}_{\text{diag}} \) arises from the implementation of fixed-angle rotations in \( \hat{H}_{\text{eff}} \) along the \( \hat{y} \) axis. Considering that such rotations do not influence the
eigenvalues of a matrix, this distinction enables the development of a mathematical framework for determining the eigenvalues of matrices that fulfill the specifications detailed in Appendix E. Consequently, this approach also facilitates the derivation of the subsequent mathematical equation.

For any integer or half integer I, the math equation below is generated during setting up the recursion relation:

\[
\left( \sqrt{\pm a^2 + 4b^2} \right)^{2I+1} \prod_{f=-I}^{I} f
\]

\[
= \sum_{k=0}^{\left\lfloor \frac{2I+1}{2} \right\rfloor} \sum_{c_1=1}^{2I-2(k-1)} \sum_{c_2=c_1+2}^{2I-2(k-2)} \cdots \sum_{c_k=c_{k-1}+2}^{2I} \left[ \prod_{j=1}^{k} \frac{1}{(I+1-c_j)(I-c_j)} a^{2I+1-2k} b^{2k} \prod_{L_i=-I}^{I} L_i \right]
\]

(3.32)

Where, \(a\) and \(b\) can be any number, \(\left\lfloor \frac{2I+1}{2} \right\rfloor\) means the floor operator, for examples, \(\left\lfloor \frac{3}{2} \right\rfloor = 1\), and \(\left\lfloor \frac{4}{2} \right\rfloor = 2\). The detailed derivation shown in APPENDIX E.

Finding the State Function for Nuclei

Based on \(\hat{H}_{\text{diag}} = \Omega_n I_z\) and the Schrödinger equation, the diagonalized state function can be written as

\[
\hat{H}_{\text{diag}} |\psi''(t)\rangle = \Omega_n I_z |\psi''(t)\rangle = i\hbar \frac{\partial |\psi''(t)\rangle}{\partial t}
\]

(3.33)

Therefore,

\[
|\psi''(t)\rangle = e^{-i\Omega_n I_z t / \hbar} |\psi''(0)\rangle
\]

(3.34)
Based on $\hat{H}_{\text{eff}} = (\omega_{n0} - \omega) I_z + \omega_{n1} I_x$, and the Schrödinger equation, the state function $|\psi'(t)\rangle$ can be written as

$$\hat{H}_{\text{eff}} |\psi'(t)\rangle = \left[(\omega_{n0} - \omega) I_z + \omega_{n1} I_x\right] |\psi'(t)\rangle$$

$$= \left[e^{-i\beta_n I_y/\hbar} \Omega_n I_z e^{i\beta_n I_y/\hbar}\right] |\psi'(t)\rangle$$

$$= i\hbar \frac{\partial |\psi'(t)\rangle}{\partial t} \tag{3.35}$$

Therefore, the Schrödinger equation can have a reasonable trial solution:

$$|\psi'(t)\rangle = e^{-i\beta_n I_y/\hbar} e^{-i\Omega_n I_z t/\hbar} e^{i\beta_n I_y/\hbar} |\psi'(0)\rangle$$

Which match with the Fig. 3.1, part (a) to part (b) doing a clockwise rotation along the $\hat{y}$ axis, then part (b) to part (c) doing a clockwise rotation along the $\hat{z}$ axis, at last part (c) to part (d) doing a counterclockwise rotation along the $\hat{y}$ axis.

Checking the trial solution by putting the solution into the left side of the Schrödinger equation,

$$\hat{H}_{\text{eff}} |\psi'(t)\rangle = e^{-i\beta_n I_y/\hbar} \Omega_n I_z e^{i\beta_n I_y/\hbar} e^{-i\Omega_n I_z t/\hbar} e^{i\beta_n I_y/\hbar} |\psi'(0)\rangle$$

$$= e^{-i\beta_n I_y/\hbar} \Omega_n I_z e^{-i\Omega_n I_z t/\hbar} e^{i\beta_n I_y/\hbar} |\psi'(0)\rangle \tag{3.37}$$

Put the trial solution into the right side of the Schrödinger equation

$$i\hbar \frac{\partial |\psi'(t)\rangle}{\partial t} = i\hbar \frac{\partial}{\partial t} \left[e^{-i\beta_n I_y/\hbar} e^{-i\Omega_n I_z t/\hbar} e^{i\beta_n I_y/\hbar} |\psi'(0)\rangle\right]$$

$$= i\hbar e^{-i\beta_n I_y/\hbar} \left[\frac{\partial}{\partial t} e^{-i\Omega_n I_z t/\hbar}\right] e^{i\beta_n I_y/\hbar} |\psi'(0)\rangle$$

$$= e^{-i\beta_n I_y/\hbar} \Omega_n I_z e^{-i\Omega_n I_z t/\hbar} e^{i\beta_n I_y/\hbar} |\psi'(0)\rangle \tag{3.38}$$

From all of the above, the left side of the Schrödinger equation equals the right side of the Schrödinger equation with the trial solution. Indeed, $|\psi'(t)\rangle = e^{-i\beta_n I_y/\hbar} e^{-i\Omega_n I_z t/\hbar} e^{i\beta_n I_y/\hbar} |\psi'(0)\rangle$ is the correct solution.
Therefore, the solution can be combined with the first rotation along the \( \hat{z} \) axis (from the line following Eqn. (3.14)), the initial state function in the rotating wave approximation can be written as

\[
|\psi(t)\rangle = |\psi_{RW A,n}(t)\rangle = e^{-i\omega I_z t/\hbar} |\psi'(t)\rangle = e^{-i\omega I_z t/\hbar} e^{-i\beta_n I_y/\hbar} e^{-i\Omega_n I_z t/\hbar} e^{i\beta_n I_y/\hbar} |\psi(0)\rangle
\]  

(3.39)

Assuming the initial state function can be rewritten as each substate \(|I, m'_j\rangle\) with the its own initial coefficient \(C_{m'}.\)

\[
|\psi(0)\rangle = \sum_{m'_j=-I}^I C_{m'}(0) |I, m'_j\rangle
\]  

(3.40)

Then the state function at the time \(t\) can be written as,

\[
|\psi(t)\rangle = \sum_{m''_j=-I}^I C_{m''}(t) |I, m''_j\rangle
\]  

(3.41)

Taking the inner product of the Eqn. (3.41) with an initial state \(|I, m_i\rangle|,\)

\[
\langle I, m_i | \psi(t) \rangle = \langle I, m_i | \sum_{m''_j=-I}^I C_{m''}(t) |I, m''_j\rangle
\]  

\[
C_{m}(t) = \sum_{m'_j=-I}^I C_{m'}(0) \langle I, m_i | e^{-i\omega I_z t/\hbar} e^{-i\beta_n I_y/\hbar} e^{-i\Omega_n I_z t/\hbar} e^{i\beta_n I_y/\hbar} |I, m'_j\rangle
\]  

(3.42)

The identity operators between each rotational matrix can be written as,

\[
\sum_{m'_j=-I}^I |I, m'_j\rangle \langle I, m'_j| = \sum_{m''_j=-I}^I |I, m''_j\rangle \langle I, m''_j| = \sum_{m'''_j=-I}^I |I, m'''_j\rangle \langle I, m'''_j|
\]  

(3.43)

\[
= \sum_{m''''_j=-I}^I |I, m''''_j\rangle \langle I, m''''_j| = 1
\]

And, \(\langle I, m_i | I, m'_j \rangle = \delta_{m_i, m'_j}\). Therefore, letting \(m_j \equiv m_i\), \(C_{m_i}(t)\) can be written as
\( C_m(t) = \sum_{m',m'',m''',m''''=-I} C_{m'}(0) \langle I, m_i | e^{-i\omega I_z t/\hbar} | I, m'' \rangle \langle I, m'' | e^{-i\beta_n I_y/\hbar} | I, m''' \rangle \langle I, m''' | e^{-i\gamma_n I_z t/\hbar} | I, m'''' \rangle = -I C_m'(0) \langle \langle I, m_i | e^{-i \omega m_i t/\hbar} | e^{-i \beta_n I_y/\hbar} | I, m' \rangle \langle I, m'' | e^{-i \beta_n I_y/\hbar} | I, m''' \rangle \langle I, m''' | e^{-i \Omega n I_z t/\hbar} | e^{i \beta_n I_y/\hbar} | I, m'''' \rangle \rangle \)

where the \( d_{m',m}^{(I)} (\beta_n) \) are the Wigner small d matrices [21, 25, 26].

\[
d^{(I)}_{m',m} (\beta_n) \equiv \langle I, m' | e^{-i\beta_n I_y/\hbar} | I, m \rangle = \sum_k (-1)^{k-m+m'} \frac{(I+m)! (I-m)! (I+m')! (I-m')!}{(I+m-k)! k! (I-k-m')! (k-m+m')} \times \left[ \cos (\beta_n/2) \right]^{2I-2k+m-m'} \left[ \sin (\beta_n/2) \right]^{2k-m+m'}
\]

where \( k \) takes on all values for which are positive and in the range, \( \max(0, m - m') \leq k \leq \min(I + m, I - m') \). Additionally,

\[
\sin (\beta_n/2) = \sqrt{\frac{1 - \cos (\beta_n)}{2}} = \sqrt{\frac{\Omega_n + \omega - \omega_n \Omega}{2\Omega_n}}
\]
\[
\cos \left( \frac{\beta_n}{2} \right) = \sqrt{\frac{1 + \cos (\beta_n)}{2}} = \sqrt{\frac{\Omega_n + \omega_{\mu 0} - \omega}{2\Omega_n}} \quad (3.47)
\]

both of the equations are finite and independent of the time \( t \).

The time dependence for equation 3.44 matches the result of Hall and Klemm, who showed the equation valid for spin \( I = \frac{1}{2}, 1, \frac{3}{2} \) cases [27], but did not calculate the constant coefficients. That \( T = 0 \) model was subsequently extended to finite \( T \) [28].

Finding the State Function of an Electron

In an atom or molecule, the electrons surrounding the nucleus can also be affected by magnetic fields applied to the sample. In addition, the electron spin matrix is identical to the nucleus. Therefore, the Hamiltonian for an electron in its surroundings can be written as

\[
\hat{H}_{RW,\text{e}} (t) = \omega_{e0} J_z + \omega_{e1} \left[ J_x \cos (\omega t) + J_y \sin (\omega t) \right] \quad (3.48)
\]

where \( \omega_{e0} = \mu_e H_0 \) and \( \omega_{e1} = \mu_e H_1 \), and the components \( J_i \) satisfy the standard Lie algebra

\[
[J_\lambda, J_\mu] = i\hbar \epsilon_{\lambda\mu\nu} J_\nu \quad (3.49)
\]

where \( \mu_e = \frac{ge}{2m_e} \quad (3.50) \)

where the mass of the electron \( m_e = 9.1093837015(28) \times 10^{-31} \text{ kg} \) [29], the charge of electron \( e \), and \( (g - 2)/2 = \frac{\alpha}{2\pi} + \cdots \) [30] which includes the complete series of quantum electrodynamics (QED) corrects ion to the magnetic moment of electron, and \( \alpha \) is the fine structure constant. The up to date calculation \( (g - 2)/2 = 1159652181.606 (11) (12) (229) \times 10^{-12} \), with three uncertainties in parentheses for the 10th order QED calculations, and the best measurement of the fine structure
constant [31]. The ratio $m_p/m_e = 1836.152673346 (81)$[32], with recently improved precision by a factor of 2 [29]. Usually, the mass of the nucleus is three to five order of magnitude heavier than the mass of the electron, therefore $\omega_{e0}$ and $\omega_{e1}$ are about three to five order of magnitude greater than $\omega_{n0}$ and $\omega_{n1}$. Even though the theory assumes the position and magnetic field strengths for the electrons and the nuclei are identical to each other, the magnetic moments for an electron and its nucleus are gratefully different due to the enormous difference in the masses of these two particles.

Therefore, the exact electronic wave function in the magnetic field can be written as

$$|\psi_{RW,A,e}(t)\rangle = e^{-iJ_z\omega t/\hbar}e^{-iJ_y\omega_0 t/\hbar}e^{-i\Omega_e J_z t/\hbar}e^{i\beta_e J_y t/\hbar}|\psi_e(0)\rangle$$

(3.51)

where

$$\sin (\beta_e) = \frac{\omega_{e1}}{\Omega_e}, \quad \cos (\beta_e) = \frac{\omega_{e0} - \omega}{\Omega_e}$$

(3.52)

$$\Omega_e = \sqrt{(\omega - \omega_{e0})^2 + \omega_{e1}^2}$$

(3.53)

Note that frequencies $\omega \approx \omega_{n0}$ can be used for nuclear magnetic resonance studies, and $\omega \approx \omega_{e0}$ can be used for electron paramagnetic resonance studies. $\omega_{e0}$ is usually three to five orders of magnitude larger than $\omega_{n0}$ depending on the mass of the corresponding nucleus.

Similar to the nuclear $\beta_n$, the electron $\beta_e$ can be defined,

$$\beta_e = \sin^{-1} \left( \frac{\omega_{e1}}{\Omega_e} \right)$$

(3.54)

The bare state function to start the perturbation calculation can be written as

$$|\Psi_{RW,A,ne}(t)\rangle = |\Psi_{RW,A,n}(t)\rangle \otimes |\Psi_{RW,A,e}(t)\rangle$$

(3.55)
\[ |\Psi_{RW A,n}(t)\rangle = e^{-i\omega t (I_z 1_e + 1_n J_z) / \hbar} e^{-i(\beta_n I_y 1_e + \beta_e 1_n J_y) / \hbar} \times e^{-i(\Omega_n I_z 1_e + \Omega_e 1_n J_z) / \hbar} e^{+i(\beta_n I_y 1_e + \beta_e 1_n J_y) / \hbar} |\Psi_{RW A,ne}(0)\rangle \quad (3.56) \]

where \( 1_e \) and \( 1_n \) are the identity matrices with ranks \( 2J + 1 \) and \( 2I + 1 \) respectively.

\[ |\Psi_{RW A,ne}(0)\rangle = \sum_{m=-I}^{I} C_m(0) |I, m\rangle \otimes \sum_{\bar{m}=-J}^{J} D_{\bar{m}}(0) |J, \bar{m}\rangle \quad (3.57) \]

and

\[ \sum_{m=-I}^{I} |C_m(0)|^2 = \sum_{\bar{m}=-J}^{J} |D_{\bar{m}}(0)|^2 = 1 \quad (3.58) \]

to force the normalization.

### Adiabatic Approximation

In the adiabatic approximation [21, 25, 26, 33], the states cannot transition from one state to another. Therefore,

\[ C_{m}^{ad}(t) = C_m(0) e^{-im\omega t} e^{-im\Omega t} |d_{m,m}^{(I)}(\beta)|^2 \quad (3.59) \]

and

\[ D_{\bar{m}}^{ad}(t) = D_{\bar{m}}(0) e^{-i\bar{m}\omega t} e^{-i\bar{m}\Omega t} |d_{m,\bar{m}}^{(I)}(\beta)|^2 \quad (3.60) \]
which can be rewritten as [21, 25, 26, 33]

\[ C^{ad}_m (t) = e^{i\theta_m(t)} e^{i\gamma_m(t)} C^{ad}_m (0) \]  

(3.61)

and

\[ D^{ad}_{\bar{m}} (t) = e^{i\theta_{\bar{m}}(t)} e^{i\gamma_{\bar{m}}(t)} D^{ad}_{\bar{m}} (0) \]  

(3.62)

For calculating the dynamic phase and the geometric phase need to redefine the setting in Eqn.(3.2), Eqn.(3.48), Eqn.(3.30), and Eqn.(3.53). Letting \( \omega_{n0} \rightarrow \omega_{n0} \cos \alpha_n \), \( \omega_{n1} \rightarrow \omega_{n0} \sin \alpha_n \), \( \omega_{e0} \rightarrow \omega_{e0} \cos \alpha_e \), and \( \omega_{e1} \rightarrow \omega_{e0} \sin \alpha_e \). Therefore, the magnetic field \( H(t) \) can sweep on a circular path about the \( \hat{z} \) axis with small tilt angles \( \alpha_n \) and \( \alpha_e \)[25].

The dynamic phases can be written as \( \theta_m (t) = -m\omega_{n0}t \) for nuclear, and \( \theta_{\bar{m}} (t) = -\bar{m}\omega_{e0}t \) for electron by integrating \( -E_m/\hbar = -m\omega_{n0}t \) and \( -E_{\bar{m}}/\hbar = -\bar{m}\omega_{e0}t \), where \( E_m \) and \( E_{\bar{m}} \) are the energies from the \( m \) and \( \bar{m} \) states from Eqn.(3.2) and Eqn.(3.48) with setting for \( \omega_{n0}, \omega_{n1}, \omega_{e0}, \) and \( \omega_{e1} \) in the \( \omega \rightarrow 0 \) limit [21, 25, 26, 33]. The expression for \( \theta_m (t) \) and \( \theta_{\bar{m}} (t) \) are in the much lower \( \omega \) range than for both resonance, \( \omega \ll \omega_{n0}, \omega_{e0} \).

The geometric (or Berry) phase \( \gamma_m (t) \) and \( \gamma_{\bar{m}} (t) \) can be obtained by Eqn. (3.59), Eqn. (3.60), Eqn. (3.61), and Eqn. (3.62). At \( t = T_0 = \frac{2\pi}{\omega} \), the period of slow sweeping motion equals the time for a complete closed geometrical orbit.

\[ \gamma_m (T_0) = -m (\omega + \Omega_n) T_0 - \theta_m (T_0) \approx 2\pi m (\cos \alpha_n - 1) \]  

(3.63)

\[ \gamma_{\bar{m}} (T_0) = -\bar{m} (\omega + \Omega_e) T_0 - \theta_{\bar{m}} (T_0) \approx 2\pi \bar{m} (\cos \alpha_e - 1) \]  

(3.64)

which apply for \( m \) and \( \bar{m} \) from \(-I \) to \( I \) and \(-J \) to \( J \) respectively. The results agrees with the
standard result for $I, J = \frac{1}{2}$ [21, 25, 26, 33] and agreed with general result for $-I \geq m \geq I$ and $-J \geq \bar{m} \geq J$ [26]. Additionally, $\theta_0(t) = \gamma_0(T_0) = 0$ when $m = 0$.

Occupation Probabilities and Resonance

For nuclear spins, interchanging $m$ and $m'$ in Eqn. (3.42),

$$1 = \langle \psi_{RW,A,n}(t) | \psi_{RW,A,n}(t) \rangle = \sum_{m'=-I}^{I} P_{m'}(t)$$

(3.65)

where,

$$P_{m'}(t) = |C_{m'}(t)|^2$$

(3.66)

is the probability of the occupation of eigenstate $|I, m'\rangle$. The sums in Eqn. (3.66) has the range $-I \geq m'' \geq I$. $I$ can be integer spin or half integer spin. For making comparison with Gottfried’s result [14], in which only $|I, m\rangle$ state is initially occupied,

$$C_{m'''}(0) = \delta_{m,m''}$$

(3.67)

Therefore,

$$P_{m'}(t) = \left| \sum_{m''=-I}^{I} e^{-im''\Omega_n t} d_{m,m''}^{(I)}(\beta_n) d_{m,m''}^{(I)*}(\beta_n) \right|^2$$

(3.68)

Compare to Gottfried’s solution in Eqn. (2.26), Eqn. (3.68) marched the result with Gottfried’s formula for general single state to single state cases. However, Gottfried’s equation unable to calculate any mixer state to any mixer state, single state to any mixer state, or any mixer state to a single state cases. The Gottfried’s Eqn. (2.26) do not allowed any phase shift at initial states, but the Eqn. (3.68) not only allowed the phase shift at the initial states also allowed to calculate any
entangled states. More detailed numerical graphic comparison can be found in Chapter 4 Section 4.

The probability function $P_{m'}$ in equation 3.68 explicitly detailed the periodic behavior with time,

$$ T_n = \frac{2\pi}{\Omega_n} \tag{3.69} $$

The time dependence results are consistent with that Hall and Klemm obtained for the $I = \frac{1}{2}, 1, \frac{3}{2}$ cases [27]. The spin $\frac{1}{2}$ case is also consistent with Gottfried's result in equation 2.27 [14].

For electronic total angular momentum states, by interchanging $m'$ and $\bar{m}'$ and substitute $n$ and $e$, equation (3.66) becomes

$$ P_{\bar{m}'} = |\tilde{D}_{\bar{m}'}(t)|^2 $$

$$ = \left| \sum_{\tilde{m}'', \tilde{m}'''} \bar{D}_{\tilde{m}'', \tilde{m}'''}(0) e^{-i\tilde{m}''\Omega_e t} d^{(I)}_{\tilde{m}'', \tilde{m}'''}(\beta_e) d^{(I)*}_{\tilde{m}'', \tilde{m}'''}(\beta_e) \right|^2 \tag{3.70} $$

Perturbations with the RWA Hamiltonian

For atomic particles which has spin number $\geq 1$, the nucleus also have an electric quadrupole moment which could play a rule in NMR measurements [18, 19, 34]. In many cases, the electric quadrupole moment could broaden the NMR transition. For example, $^{14}$N has a 99.6% natural abundance, but it has been difficult to observed in NMR experiments due to the broadening effect by the electric quadrupole moment. However, recent discoveries found that $^{14}$N samples could be detected when dissolved in a variety of solvents [35–38]. $^{14}$N is essential isotope in the nucleic amino acids cytosine, guanine, adenine, uracil, and thymine within the DNA and RNA molecules. The table 3.1 contains a list of dipole and quadrupole moments of comment isotopes. In the first-row atoms [39–43], the interaction of the electrons with the nucleus gives rise to hyperfine struc-
ture in the electronic atomic structure. Hund’s rules for the electronic state hieroglyphic notation $^{2S+1}L_J$, [25, 44] along with the overall antisymmetry of the electronic states for an odd number of electrons, which only fill the $n = 1$ and partially fill the $n = 2$ atomic level states, the electronic ground state for atomic N is $^4S_{\frac{3}{2}}$ and the excited states energy are $^2D_{\frac{5}{2}}, ^2D_{\frac{3}{2}}, ^2P_{\frac{1}{2}}, ^2P_{\frac{3}{2}}$, and $^2S_{\frac{1}{2}}$. Thus, there are 6 low-lying electronic states of N with $J = \frac{5}{2}, \frac{3}{2},$ and $\frac{1}{2}$.

Table 3.1: The Properties of The Stable Isotopes

<table>
<thead>
<tr>
<th>Isotope</th>
<th>I</th>
<th>P</th>
<th>$\mu_n/\mu_N$</th>
<th>Q(b)</th>
<th>atomic%</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^1$H</td>
<td>1/2</td>
<td>+</td>
<td>+2.79284734(3)</td>
<td></td>
<td>99.985</td>
</tr>
<tr>
<td>$^2$H</td>
<td>1</td>
<td>+</td>
<td>+0.85743822(9)</td>
<td>+0.00285783(30)</td>
<td>0.0135</td>
</tr>
<tr>
<td>$^{13}$C</td>
<td>1/2</td>
<td>-</td>
<td>+0.7024118(14)</td>
<td></td>
<td>1.1</td>
</tr>
<tr>
<td>$^{14}$N</td>
<td>1</td>
<td>+</td>
<td>+0.40376100(6)</td>
<td>+0.02044(3)</td>
<td>99.6</td>
</tr>
<tr>
<td>$^{15}$N</td>
<td>1/2</td>
<td>-</td>
<td>-0.28318884(5)</td>
<td></td>
<td>0.38</td>
</tr>
<tr>
<td>$^{17}$O</td>
<td>5/2</td>
<td>+</td>
<td>-1.89379(9)</td>
<td>-0.02558(22)</td>
<td>0.037</td>
</tr>
<tr>
<td>$^{29}$Si</td>
<td>1/2</td>
<td>+</td>
<td>-0.55529(3)</td>
<td></td>
<td>4.67</td>
</tr>
<tr>
<td>$^{31}$P</td>
<td>1/2</td>
<td>+</td>
<td>+1.13160(3)</td>
<td></td>
<td>100</td>
</tr>
<tr>
<td>$^{33}$S</td>
<td>3/2</td>
<td>+</td>
<td>+0.6438212(14)</td>
<td>-0.0694(4)</td>
<td>0.75</td>
</tr>
<tr>
<td>$^{43}$Ca</td>
<td>7/2</td>
<td>-</td>
<td>-1.3173(6)</td>
<td>-0.408(8)</td>
<td>0.135</td>
</tr>
<tr>
<td>$^{57}$Fe</td>
<td>1/2</td>
<td>-</td>
<td>+0.0906</td>
<td></td>
<td>2.119</td>
</tr>
<tr>
<td>$^{87}$Sr</td>
<td>9/2</td>
<td>+</td>
<td>-1.0936030(13)</td>
<td>+3.05(2)</td>
<td>7.00</td>
</tr>
</tbody>
</table>

TABLE 3. Table of the stable isotopes, spin quantum numbers, $I$, parity $P$, nuclear magnetic moments $\mu_n$ relate to the unclear magneton $\mu_N = (e\hbar) / (2m_p) = 5.05783699(31) \times 10^{-27} J/T$, the
The electronic quadrupole moment $Q$ in barns ($1 \text{ barn} = 10^{-28} \text{m}^2$), and atomic % abundance [15, 16, 34]. The atoms in adenine, cytosine, guanine, thymine, and uracil. Three isotopes of possible chemical defect substitutions, Si, P, and S, respectively for C, N, and O, and three isotopes present in blood and bones.

For calculation of atoms, the low-lying states can be accurately predicted by assuming the electronic nuclear moment can be represented by the corresponding $J$ value and the related energy levels. Molecular structures like the nucleic amino acids in DNA and RNA could have several quantized electronic angular momentum value, which could be more complex for calculations.

The nuclear electric quadrupole moment appears when the nuclear spin number $I \geq 1$, and electron spin number $J \geq \frac{1}{2}$. In which, the electric quadrupole moment terms proportional to three electric field gradients, $\frac{\partial E}{\partial x_j}$, are anisotropic. The process was treated by perturbation using the standard interaction representation. It started with the time-independent magnetic field Hamiltonian $H_0 = \mu N I_z$ [45]. However, Gottfried emphasized that the treatment cannot work at or near resonance [14].

For solving for atoms, assuming the nuclear total angular momentum states $|I, m\rangle$ with $-I \leq m \leq I$ and $I^2$ and $I_z$ satisfy,

\[
I^2 |I, m\rangle = \hbar^2 I (I + 1) |I, m\rangle
\]
\[
I_z |I, m\rangle = \hbar m |I, m\rangle
\]  \hspace{1cm} (3.71)

with $-I \leq m \leq I$, and the analogous electronic states $|J, \bar{m}\rangle$ with $-J \leq \bar{m} \leq J$ satisfy,

\[
J^2 |J, \bar{m}\rangle = \hbar^2 J (J + 1) |J, \bar{m}\rangle
\]
\[
J_z |J, \bar{m}\rangle = \hbar \bar{m} |J, \bar{m}\rangle
\]  \hspace{1cm} (3.72)

and, both spin $I$ and $J$ operators obey the Lie algebras in equations (3.5) and (3.49). And the nuclear spin $I$ and electronic spin $J$ are independent of each other as assumed in the literature [39–43]. In the early atomic hyperfine structure calculations of first row atoms, the electronic total
angular momentum $J$ is coupled with the nuclear spin $I$ in powers of $I \cdot J$ [39–43]. The nuclear-electronic dipole-dipole, electron quadrupole, and magnetic octupole interactions are listed below. The nuclear-electronic dipole to dipole Hamiltonian can be written as

$$H_D = A(I, J) I \cdot J / \hbar^2$$  \hspace{1cm} (3.73)$$

The nuclear-electronic electric quadrupole Hamiltonian can be written as

$$H_Q = B(I, J) \left[ (I \cdot J / \hbar^2)^2 + \frac{1}{2} (I \cdot J / \hbar^2)^2 - \frac{1}{3} I (I + 1) J (J + 1) \right]$$  \hspace{1cm} (3.74)$$

The corresponding magnetic octupole Hamiltonian can be written as

$$H_O = C(I, J) \left[ (I \cdot J / \hbar^2)^3 + 2 (I \cdot J / \hbar^2)^3 + \frac{1}{5} (I \cdot J / \hbar^2)^3 \right] - 3 I (I + 1) J (J + 1)$$

$$+ I (I + 1) J (J + 1) + 3] - 5 I (I + 1) J (J + 1)$$  \hspace{1cm} (3.75)$$

These are respectively proportional to linear, quadratic, and cubic functions of $(I \cdot J)$. In addition $A(I, J)$, $B(I, J)$, and $C(I, J)$ are the energy coefficients for the magnetic dipole, electric quadrupole, and magnetic octupole moments, respectively. They also contain the integrations over the nuclear and electronic structural variables in the $|I, I\rangle \times |J, J\rangle$ state factor due to the Wigner-Eckart theorem [18, 19, 43, 46]. Similarly, the electric hexadecapole moment can be written as a quartic function of $(I \cdot J)$ [18, 43, 46].

The nuclear moment perturbations were studied without an applied magnetic field in the past, to include their effects upon the atomic hyperfine structure of atom [39–43]. In those cases, the operators $I$, $J$, and combined $F = I + J$ gave good quantum numbers. And the nuclear moment perturbations could be written in terms of the single quantum number $K = F (F + 1)$ [39–43]. However, the three components of RWA applied magnetic fields will break the symmetry in all directions, but the scalar operator $I \cdot J$ is well defined, provided that $I$ and $J$ are both good quantum
numbers.

Starting with the RWA for the nuclei and electronic cloud of an atom, assuming the full Hamiltonian can be written as

\[ \hat{H}(t) = \hat{H}_n(t) \otimes \mathbf{1}_e + \mathbf{1}_n \otimes \hat{H}_e(t) + \hat{H}_{ne} \quad (3.76) \]

\[ \hat{H}_n(t) = \hat{H}_{RW,n}(t) + \hat{V}_n(t) \quad (3.77) \]

\[ \hat{H}_e(t) = \hat{H}_{RW,e}(t) + \hat{V}_e(t) \quad (3.78) \]

\[ \hat{H}_{ne} = \sum_{q=0}^{2I} K_q(I, J) \left[ \mathbf{I} \cdot \mathbf{J}/\hbar^2 \right]^q \mathbf{1}_n \otimes \mathbf{1}_e \quad (3.79) \]

where the \( K_q(I, j) \) are energies that are real functions of \( I \) and \( J \). The bare Hamiltonian matched the Hamiltonian in equation 3.2 for \( \hat{H}_{RW,n}(t) \) and equation 3.48 for \( \hat{H}_{RW,e}(t) \).

The calculation for \( \mathbf{I} \cdot \mathbf{J} \) can be achieved by using tensor algebra \( |I, m_I⟩ \otimes |J, m_J⟩ \). The combined RWA Hamiltonian can be represented by a rank \((2I + 1)\) matrix for the nuclear operators multiply a rank \((2J + 1)\) matrix for the surrounding electron cloud into a rank \((2I + 1)(2J + 1)\) matrix. However, an atom could potentially have multiple \( J \) values. Therefore, the calculation could potentially have multiple rank \((2I + 1)(2J + 1)\) matrices with different \( J \) values. Here, the Hamiltonian does not include different \( I \) values for different isotopes, or the interaction within molecules. For example, \( J - J \) couplings, \( I - J - I \) coupling, lattice structures, etc, can be important. In future research, the incorporation of these types of situations into calculations is planned, whereas the current focus is solely on the atomic and diatomic molecules cases.

It is easy to show that the full \( |\psi_{RW,ne}(t)⟩ \) including both electrons and nuclei in atoms satisfies the Schrödinger equation for the total RWA Hamiltonian,

\[ \hat{H}_{RW,ne}(t) = \hat{H}_{RW,n}(t) \otimes \mathbf{1}_e + \mathbf{1}_n \otimes \hat{H}_{RW,e}(t) \quad (3.80) \]
There are two types of perturbations considered here. The periodic time-dependent perturbation included by the experimental applied magnetic field. the second one is the time-independent perturbation due to the nuclear spin $I$ interacting with its surrounding electron spin $J$.

Based on the type of the experiment, the time dependent perturbations can be separated into the experimental time-dependent field and into the RWA time-dependent field.

For a general time-dependent field form in the $xy$ plane, the perturbation can be written as

$$
\delta \hat{V}_1 (t) = \delta \hat{V}_{n1} (t) \otimes \mathbf{1}_e + \mathbf{1}_n \otimes \delta \hat{V}_{e1} (t)
$$

(3.82)

$$
\delta \hat{V}_{n1} (t) = -\omega_{n1} I_y \sin (\omega t) + \omega_{n1} I_x \sum_{p=2}^{\infty} a_p \cos [p \omega (t - t_0)]
$$

(3.83)

$$
\delta \hat{V}_{e1} (t) = -\omega_{e1} J_y \sin (\omega t) + \omega_{e1} J_x \sum_{p=2}^{\infty} a_p \cos [p \omega (t - t_0)]
$$

(3.84)

where any wave form can be calculated by using Fourier series [47].

For the magic-angle spinning case can be written as [48],

$$
\delta \hat{V}_2 (t) = \delta \hat{V}_{n2} (t) \otimes \mathbf{1}_e + \mathbf{1}_n \otimes \delta \hat{V}_{e2} (t)
$$

(3.85)

$$
\delta \hat{V}_{n2} (t) = 2\omega_{n1} I_y \sin \theta \cos (\omega t) (I_z \cos \theta - I_x \sin \theta)
$$

(3.86)

$$
\delta \hat{V}_{e2} (t) = 2\omega_{e1} J_y \sin \theta \cos (\omega t) (J_z \cos \theta - J_x \sin \theta)
$$

(3.87)

For the above two experiments, the full perturbation can also be written as

$$
\delta \hat{V}_i (t) = \delta \hat{V}_{ni} (t) \otimes \mathbf{1}_e + \mathbf{1}_n \otimes \delta \hat{V}_{ei} (t) + \delta \hat{V}_{n,e}
$$

(3.88)

$$
\delta \hat{V}_{n,e} = \sum_{q=0}^{2I} K_q (\mathbf{1} \cdot \mathbf{J} / \hbar^2)^q \mathbf{1}_n \otimes \mathbf{1}_e
$$

(3.89)
In this context, \( i = 1, 2 \) corresponds to the two aforementioned experiments. The \( K_q \) functions depend on the quantum numbers \( I \) and \( J \), along with the constants from the nuclear and electronic wave functions evaluated in the \( |I, I\rangle \) and \( |J, J\rangle \) states, as determined by the Wigner-Eckart theorem [43]. Interactions between nuclear and electron components within diatomic molecules, encompassing magnetic dipole moments, electric quadrupole moments, magnetic octupole moments, and hexadecapoles, among others, can be expressed as functions of \( \mathbf{I} \cdot \mathbf{J} \). This term, \( \mathbf{I} \cdot \mathbf{J} \), is a scalar, as detailed in [39–43], and is comprehensively described by equation 3.89.

Let’s proceed to calculate the perturbation due to \( \delta \hat{V}_i(t) \), assuming

\[
|\psi_{ne}(t)\rangle = |\psi_{RW,ne}(t)\rangle + \lambda |\psi_{1,ne}(t)\rangle + \lambda^2 |\psi_{2,ne}(t)\rangle + \cdots
\]

\( \hat{H}_{ne}(t) = \hat{H}_{RW,ne}(t) + \lambda \delta \hat{V}_i(t) \) (3.90)

Each of the \( \lambda \) terms should satisfy the Schrödinger equation

\[
i\hbar \frac{\partial}{\partial t} |\psi_{k,ne}(t)\rangle = \hat{H}_{ne}(t) |\psi_{k,ne}(t)\rangle
\] (3.91)

To \( k \)-th order in \( \lambda \).

When \( k = 0 \),

\[
i\hbar \frac{\partial}{\partial t} |\psi_{RW,ne}(t)\rangle = \hat{H}_{RW,ne}(t) |\psi_{RW,ne}(t)\rangle
\] (3.92)

When \( k = 1 \),

\[
i\hbar \frac{\partial}{\partial t} |\psi_{1,ne}(t)\rangle = \hat{H}_{RW,ne}(t) |\psi_{1,ne}(t)\rangle + \delta \hat{V}_i(t) |\psi_{RW,ne}(t)\rangle
\] (3.93)

When \( k > 1 \),
\( i \hbar \frac{\partial}{\partial t} |\psi_{k,ne} (t)\rangle = \tilde{H}_{RW,A,ne} (t) |\psi_{k,ne} (t)\rangle + \delta \tilde{V}_i (t) |\psi_{k-1,ne} (t)\rangle \) (3.94)

For \( \lambda^0 \) term,

\[ e^{i(\beta_1 I_y 1_e + \beta_1 I_y 1_n J_y) / \hbar} e^{i \omega t (I_z 1_e + I_n J_z) / \hbar} \left( \frac{i \hbar}{\partial t} \right) e^{-i \omega t (I_z 1_e + I_n J_z) / \hbar} \]

\[ \times e^{-i(\beta_1 I_y 1_e + \beta_1 I_y 1_n J_y) / \hbar} e^{i(\beta_1 I_y 1_e + \beta_1 I_y 1_n J_y) / \hbar} e^{i \omega t (I_z 1_e + I_n J_z) / \hbar} |\psi_{RW,A,ne} (t)\rangle \]

\[ = e^{i(\beta_1 I_y 1_e + \beta_1 I_y 1_n J_y) / \hbar} e^{i \omega t (I_z 1_e + I_n J_z) / \hbar} H_{RW,A,ne} (t) e^{-i \omega t (I_z 1_e + I_n J_z) / \hbar} e^{-i(\beta_1 I_y 1_e + \beta_1 I_y 1_n J_y) / \hbar} \]

\[ \times e^{i(\beta_1 I_y 1_e + \beta_1 I_y 1_n J_y) / \hbar} e^{i \omega t (I_z 1_e + I_n J_z) / \hbar} |\psi_{RW,A,ne} (t)\rangle \] (3.95)

where \( \tilde{H}_{RW,A,ne} (t) \) is given by equations (3.2), (3.48), and (3.55). Therefore, the equation above can be written as,

\[ i \hbar \frac{\partial}{\partial t} |\tilde{\psi}_{RW,A,ne} (t)\rangle = \tilde{H}_{RW,A,ne} (t) |\tilde{\psi}_{RW,A,ne} (t)\rangle \] (3.96)

where

\[ \tilde{\psi}_{RW,A,ne} (t) = e^{i(\beta_1 I_y 1_e + \beta_1 I_y 1_n J_y) / \hbar} e^{i \omega t (I_z 1_e + I_n J_z) / \hbar} \left( \frac{\partial}{\partial t} \right) e^{-i \omega t (I_z 1_e + I_n J_z) / \hbar} e^{-i(\beta_1 I_y 1_e + \beta_1 I_y 1_n J_y) / \hbar} \]

\[ \times \tilde{H}_{RW,A,ne} (t) e^{-i \omega t (I_z 1_e + I_n J_z) / \hbar} e^{-i(\beta_1 I_y 1_e + \beta_1 I_y 1_n J_y) / \hbar} \] (3.97)

\[ |\tilde{\psi}_{RW,A,ne} (t)\rangle = e^{i(\beta_1 I_y 1_e + \beta_1 I_y 1_n J_y) / \hbar} e^{i \omega t (I_z 1_e + I_n J_z) / \hbar} |\psi_{RW,A,ne} (t)\rangle \]

which is equivalent to the total Schrödinger equation.

\[ i \hbar \frac{\partial}{\partial t} |\tilde{\psi}_{RW,A,ne} (t)\rangle = \tilde{H}_0 |\tilde{\psi}_{RW,A,ne} (t)\rangle \] (3.100)
and the time-independent bare Hamiltonian $\hat{H}_0$ given by

$$\hat{H}_0 = \Omega_n I_z \otimes 1_e + \Omega_e 1_n \otimes J_z$$  (3.101)

Based on equations (3.55) and (3.99)

$$|\tilde{\psi}_{RW A, ne}(t)\rangle = e^{-i\left(\Omega_n I_z + \Omega_e J_z\right)/\hbar} e^{i\left(\beta_n I_y 1_e + \beta_e 1_n J_y\right)/\hbar} |\psi_{RW A, ne}(0)\rangle$$

$$= e^{-i\hat{H}_0 t/\hbar} |\psi_{RW A, ne,r}(0)\rangle_S$$

The Schrödinger picture contains the doubly-rotated wave function,

$$|\psi_{RW A, ne,r}(0)\rangle_S = e^{i(\beta_n I_y 1_e + \beta_e 1_n J_y)/\hbar} |\psi_{RW A, ne}(0)\rangle$$  (3.103)

The original laboratory frame given by Eqn. (3.57) leads to a complicated expression for the ground state energy, therefore the calculation should change the basis to the doubly rotated frame in the Schrödinger picture. Letting

$$|\psi_{RW A, ne,r}(0)\rangle_S \equiv \sum_{m=-I}^{I} \sum_{\bar{m}=-J}^{J} \tilde{C}_m(0) \tilde{D}_{\bar{m}}(0) |I, m\rangle \otimes |J, \bar{m}\rangle$$  (3.104)

where can be normalized by

$$\sum_{m=-I}^{I} \left| \tilde{C}_m(0) \right|^2 = \sum_{\bar{m}=-J}^{J} \left| \tilde{D}_{\bar{m}}(0) \right|^2 = 1$$  (3.105)

The coefficients $\tilde{C}_m(0)$ and $\tilde{D}_{\bar{m}}(0)$ in the doubly-rotated new basis are given by
\[ \tilde{C}_m (0) = \sum_{m'=-I}^{I} \langle I, m | e^{i\beta_n I_y/\hbar} | I, m' \rangle C_{m'} (0) \]
\[ = \sum_{m'=-I}^{I} d^{(I)\ast}_{m,m'} (\beta_n) C_{m'} (0) \]  
\[ \tilde{D}_{\bar{m}} (0) = \sum_{\bar{m}'=-J}^{J} \langle J, \bar{m} | e^{i\beta_e J_y/\hbar} | J, \bar{m}' \rangle D_{\bar{m}'} (0) \]
\[ = \sum_{\bar{m}'=-J}^{J} d^{(J)\ast}_{\bar{m},\bar{m}'} (\beta_e) D_{\bar{m}'} (0) \]  

where \( d^{(f)\ast}_{m',m} (\beta_n) \) is given by the Wigner small-d matrix \([21, 25, 26]\), and presented in Eqn. (3.45).

In here, \( d^{(J)\ast}_{\bar{m},\bar{m}'} (\beta_e) \) obtained from \( d^{(f)\ast}_{m',m} (\beta_n) \) by appropriate substitutions and complex conjugation.

In the doubly rotated-basis, the energy of the unperturbed state can be written as

\[ \tilde{E}^{(0)}_{ne} (m, \bar{m}) = \hbar (m\Omega_n + \bar{m}\Omega_e) \]  

The general form of unperturbed state energy can be written as

\[ \tilde{E}^{(0)}_{ne} = \hbar \left( \Omega_n \sum_{m=-I}^{I} m \left| \tilde{C}_m (0) \right|^2 + \Omega_e \sum_{\bar{m}=-J}^{J} \bar{m} \left| \tilde{D}_{\bar{m}} (0) \right|^2 \right) \]  

For the \( k \)-th order term, the perturbed state in Eqn. (3.94) can be written as

\[ \hbar \frac{\partial}{\partial t} | \tilde{\psi}_{k,ne} (t) \rangle = \tilde{H}_{RW,A,ne} (t) | \tilde{\psi}_{k,ne} (t) \rangle + \delta \tilde{V}_i (t) | \tilde{\psi}_{k-1,ne} (t) \rangle \]  

where

\[ | \tilde{\psi}_{k,ne} (t) \rangle = e^{i(\Omega_n I_z 1_e + \Omega_e 1_n J_z)/\hbar} e^{i(\beta_e I_y 1_e + \beta_e I_n J_y)/\hbar} | \tilde{\psi}_{k,ne} (0) \rangle \]
\[ \delta \tilde{V}_i (t) = e^{i(\beta_n I_y 1_e + \beta_e I_n J_y)/\hbar} e^{i\omega t (I_z 1_e + 1_n J_z)/\hbar} \delta \tilde{V}_i (t) e^{-i\omega t (I_z 1_e + 1_n J_z)/\hbar} e^{-i(\beta_n I_y 1_e + \beta_e I_n J_y)/\hbar} \]
where the expressions for the $\delta \hat{V}_i(t)$ are given in Appendix H.

**Nuclear Moment Perturbations in Atoms**

In recent years, there has been increased interest in the measurement of atomic nuclear moments, with a significant amount of work done for the measurements of the electric quadrupole moment and the magnetic octupole moment [49–64]. Here, a new experimental method can be proposed that could lead to improved accuracy of such moment measurements.

The untransformed nuclear moment interactions can be written as

$$
\delta \hat{V}_{ne} = \sum_{q=0}^{2I} K_q \left( \vec{I} \cdot \vec{J} / \hbar^2 \right)^q
$$

(3.112)

where

$$
\vec{I} \cdot \vec{J} = I_z J_z + \frac{1}{2} (I_+ J_- + I_- J_+)
$$

(3.113)

where $J_\pm = J_x \pm i J_y$ and $I_\pm = I_x \pm i I_y$. $I$ and $J$ have to be the good quantum numbers for which the entire infinite set of the transformed nuclear interactions are independent of $t$, and can be solved to arbitrary order in perturbation theory in principle. The transformed nuclear moment interactions can be written as

$$
\widetilde{\delta \hat{V}}_{ne} = e^{i(\beta_n I_y 1_e + \beta_e 1_n J_y) / \hbar} e^{i \omega t (I_z 1_e + 1_n J_z) / \hbar} \delta \hat{V}_{ne} e^{-i \omega t (I_z 1_e + 1_n J_z) / \hbar} e^{-i(\beta_n I_y 1_e + \beta_e 1_n J_y) / \hbar}
$$

(3.114)

since $\vec{I} \cdot \vec{J}$ (scalar) should be invariant under uniform rotations. Therefore,

$$
e^{i \omega t (I_z 1_e + 1_n J_z) / \hbar} (\vec{I} \cdot \vec{J}) e^{-i \omega t (I_z 1_e + 1_n J_z) / \hbar} = (\vec{I} \cdot \vec{J})
$$

(3.115)
which is time independent. The process can be done by generalizing the procedures from Eqn. (3.6) to Eqn. (3.12) for the rotated components of $I$ to components of $J$. It is also obviously true that when $I$ and $J$ are rotating about the same axis by the same angle. Then $(I \cdot J)^2$ also can be transformed by inserting

$$1_n \otimes 1_e = e^{i\omega t(I_z 1 e + I_n J_z)}/\hbar e^{-i\omega t(I_z 1 e + I_n J_z)}/\hbar$$

(3.116)

since the transformed nuclear moment interaction is time independent. Therefore, the laboratory frame wave functions can be doubly-rotated for calculation.

The first order energy $\tilde{E}_{ne}^{(1)}$ can be evaluated in the doubly-rotated frame in Eqn. (3.104) which is given by

$$|\tilde{\psi}_{0,ne,r}(0)\rangle = |\psi_{RW_A,ne,r}\rangle_S$$

(3.117)

The first-order perturbation for the nuclear moment interactions can be written as

$$\tilde{E}_{ne}^{(1)} = S \langle \psi_{0,ne,r}(0)|\delta \hat{V}_{ne}|\psi_{0,ne,r}(0)\rangle_S$$

(3.118)

where $\delta \hat{V}_{ne}$ is given by Eqn. (3.112). Note, that the operations of $I_z, J_z, I_\pm,$ and $J_\pm$ present in equation 3.113 are given by [14, 21, 26]

$$I_z |I, m\rangle = m\hbar |I, m\rangle$$

$$J_z |I, \bar{m}\rangle = \bar{m}\hbar |J, \bar{m}\rangle$$

$$I_\pm |I, m\rangle = \hbar \sqrt{(I \mp m)(I \pm (m + 1))} |J, m \pm 1\rangle = \hbar a^{I}_{m,\pm} |I, m \pm 1\rangle$$

(3.120)

$$J_\pm |I, \bar{m}\rangle = \hbar \sqrt{(I \mp \bar{m})(I \pm \bar{m} + 1)} |J, \bar{m} \pm 1\rangle = \hbar a^{J}_{\bar{m},\pm} |I, \bar{m} \pm 1\rangle$$

(3.121)
Use the doubly-rotated reference frame to evaluate the perturbation to the energy arising from the magnetic dipole and electric quadrupole moments. The bare Hamiltonian $\hat{H}_0$ is diagonal and independent of $t$. Then the $q = 0, 1, 2$ terms in $\delta \hat{V}_{ne}$ can be represented by the rank $2I + 2J + 2$ matrix $\hat{M}$ with elements

$$
\left( \hat{M} \right)_{m',m}^{\bar{m}',\bar{m}} = K_0 \delta_{m',m} \delta_{\bar{m}',\bar{m}} + K_1 \left[ \delta_{m',m} \delta_{\bar{m}',\bar{m}} mm\bar{m} + \frac{1}{2} \left( \delta_{m',m-1} \delta_{\bar{m}',\bar{m}} \alpha_{m,+}^{I} \alpha_{\bar{m},-}^{J} + \delta_{m',m+1} \delta_{\bar{m}',\bar{m}} \alpha_{m,-}^{I} \alpha_{\bar{m},+}^{J} \right) \right] + K_2 \left\{ \delta_{m',m} \delta_{\bar{m}',\bar{m}} \left[ m\bar{m} \left( m\bar{m} - \frac{1}{2} \right) \right] + \frac{1}{2} \left[ I \left( I + 1 \right) - m^2 \right] \left[ J \left( J + 1 \right) - \bar{m}^2 \right] + \frac{1}{2} \left( \delta_{m',m-1} \delta_{\bar{m}',\bar{m}} \alpha_{m,+}^{I} \alpha_{\bar{m},-}^{J} \right) \right. \\
\left. \times \left[ 2m\bar{m} + m - \bar{m} - 1 \right] + \delta_{m',m+1} \delta_{\bar{m}',\bar{m}} \alpha_{m,+}^{I} \alpha_{\bar{m},+}^{J} \left[ 2m\bar{m} + m - m - 1 \right] \right] + \frac{1}{4} \left[ \delta_{m',m-2} \delta_{\bar{m}',\bar{m}} \alpha_{m,-}^{I} \alpha_{\bar{m}+1,-}^{J} \right. \\
\left. + \delta_{m',m+2} \delta_{\bar{m}',\bar{m}} \alpha_{m,-}^{I} \alpha_{\bar{m}-2,+}^{J} \right] \}
$$

(3.122)

where

$$
K_0 = -\frac{1}{3} B \left( I, J \right) I \left( I + 1 \right) J \left( J + 1 \right)
$$

$$
K_1 = A \left( I, J \right) + \frac{1}{2} B \left( I, J \right)
$$

(3.123)

$$
K_2 = B \left( I, J \right)
$$

Where $A \left( I, J \right)$ and $B \left( I, J \right)$ are given elsewhere [43]. Therefore, the equation for energy eigenvalues to first order for magnetic dipole and electric quadrupole can be written as

$$
\det \left( \hat{H}_0 + \hat{M} - E \mathbf{1}_n \otimes \mathbf{1}_e \right) = 0
$$

(3.124)
CHAPTER 4: FINDINGS

Single Atom NMR Computational Results for the Nuclear Magnetic Dipole Moment

To explore the nuclear spin states in a single atom, it is essential to understand how the probabilities of the spin states evolve over time. For example, it uses the similar conditions for building quantum gates in quantum computing. By delving into the dynamics of the spin states, mainly focusing on the situation which has equal probabilities for each state at the beginning, and the scenario which has only a single state initially. The detailed computational code for arbitrary spin state probabilities over time can be found in APPENDIX A.

![Figure 4.1: Spin I=1/2](image-url)
The Plots in figure 4.1 shows the probabilities vs \( \tau \) of the spin 1/2 cases, where \( 0 \leq \tau = t/T_n \leq 1 \). the \( P_{1/2} (\tau) \) (dotted red) and \( P_{-1/2} (\tau) \) (solid blue) for \( I = \frac{1}{2} \). In part (a), (c), and (e), initial conditions \( C_{1/2} (0) e^{-i\pi/4} = C_{-1/2} (0) = \frac{1}{\sqrt{2}} \). In (b), (d), and (f), \( C_{1/2} (0) = 1 \) and \( C_{-1/2} = 0 \). In (a) and (b), \( \omega/\omega_{n0} = 0.95 \). In (c) and (d), \( \omega/\omega_{n0} = 0.99 \). In (e) and (f), \( \omega/\omega_{n0} = 1 \). Figure 4.1 also represents the \( J = \frac{1}{2} \) and \( \tau = t/T_e \) case with \( \omega_0 \) and \( D_{\bar{m}} (0) \) instead of \( \omega_{n0} \) and \( C_{\bar{m}} (0) \).

![Diagram](image)

Figure 4.2: Spin I=1

The Plots in figure 4.2 the \( P_1 (\tau) \) (dotted black), the \( P_0 (\tau) \) (dotted red) , and \( P_{-1} (\tau) \) (solid blue)
for $I = 1$ and $0 \leq \tau = t/T_n \leq 1$. In part (a), (c), and (e), initial conditions $C_1(0)e^{-i\pi/4} = C_0(0) = C_{-1}(0) = \frac{1}{\sqrt{3}}$. In (b), (d), and (f), $C_1(0) = 1$ and $C_0 = C_{-1} = 0$. In (a) and (b), $\omega/\omega_{n0} = 0.95$. In (c) and (d), $\omega/\omega_{n0} = 0.99$. In (e) and (f), $\omega/\omega_{n0} = 1$. Figure 4.2 also represents the $J = 1$ and $\tau = t/T_e$ case with $\omega_{e0}$ and $D_m(0)$ instead of $\omega_{n0}$ and $C_m(0)$.

Figure 4.3: Spin I=3/2

The Plots in Fig. 4.3 the $P_{3/2} (\tau)$ (dotted black), the $P_{1/2} (\tau)$ (dotted red), the $P_{-1/2} (\tau)$ (solid blue), and the $P_{-3/2}$ (dotted blue) for $I = 3/2$ and $0 \leq \tau = t/T_n \leq 1$. In part (a), (c), and (e),
initial conditions \( C_{\frac{3}{2}}(0) e^{-i\pi/4} = C_{\frac{1}{2}}(0) = C_{-\frac{1}{2}}(0) = C_{-\frac{3}{2}} = \frac{1}{2} \). In \((b), (d),\) and \((f)\), \( C_{\frac{3}{2}}(0) = 1 \) and \( C_m = 0 \) for \( m \neq \frac{3}{2} \). In \((a)\) and \((b)\), \( \omega/\omega_{n0} = 0.95 \). In \((c)\) and \((d)\), \( \omega/\omega_{n0} = 0.99 \). In \((e)\) and \((f)\), \( \omega/\omega_{n0} = 1 \). Figure 4.3 also represents the \( J = 3/2 \) and \( \tau = t/T_e \) case with \( \omega e_0 \) and \( D_{\bar{m}}(0) \) instead of \( \omega_{n0} \) and \( C_m(0) \).

![Figure 4.4: Spin I=2](image)

The Plots in Fig. 4.4 the \( P_2(\tau) \) (solid black), the \( P_1(\tau) \) (dotted black), the \( P_0(\tau) \) (dotted red), the \( P_{-1}(\tau) \) (solid blue), and the \( P_{-2} \) (dotted blue) for \( I = 2 \) and \( 0 \leq \tau = t/T_n \leq 1 \). In part \((a)\),
(c), and (e), initial conditions \(C_2(0) e^{-i\pi/4} = C_1(0) = C_0(0) = C_{-1}(0) = C_{-2} = \frac{1}{\sqrt{5}}\). In (b), (d), and (f), \(C_2(0) = 1\) and \(C_m = 0\) for \(m \neq 2\). In (a) and (b), \(\omega/\omega_{n0} = 0.95\). In (c) and (d), \(\omega/\omega_{n0} = 0.99\). In (e) and (f), \(\omega/\omega_{n0} = 1\). Figure 4.4 also represents the \(J = 2\) and \(\tau = t/T_e\) case with \(\omega_{e0}\) and \(D_{\bar{m}}(0)\) instead of \(\omega_{n0}\) and \(C_m(0)\).

Based on the plots in figures 4.1, 4.2, 4.3, and 4.4 in part (a), (c), and (e) the probability of individual spin state occupations will have more dramatic changes with the phase factor when it is closer to the resonance frequency. However, in part (b), (d), and (f), the phase factor dose not affect the particle, if the initial state of the particle is in a single state regardless of the rotational frequency. Higher spin value cases from \(I = 5/2\) to \(I = 9/2\) are listed in APPENDIX F.

**Period-Averaged Occupation Probabilities Near to Resonance Computational Result**

Near to the resonance frequency, One may use the equation below to compare the time averages over one period of the occupation probabilities

\[
\bar{P}_{m,\bar{m}} = \frac{1}{T_{n,e}} \int_0^{T_{n,e}} P_{m,\bar{m}}(t) \, dt
\]  

(4.1)

Due to the complexity of the integration in equation 4.1 for the corresponding matrices, Here only present the numerical graph for each individual spin case. The related computational code can be found in APPENDIX B.
Figure 4.5: Spin $I = \frac{1}{2}$ and $0.95 \leq \frac{\omega}{\omega_{n,e}} \leq 1.05$

In Fig. 4.5 plots of $\bar{P}_m$ the time averaged probability for $I = \frac{1}{2}$ over the oscillation period at the frequency $0.95 \leq \frac{\omega}{\omega_{n,e}} \leq 1.05$. In each part, $m = \frac{1}{2}$: (dotted red), $m = -\frac{1}{2}$: (solid blue). Part (a), the initial conditions $C_{\frac{1}{2}}(0) = C_{-\frac{1}{2}}(0) = \frac{1}{\sqrt{2}}$ (equal probabilities initially without a phase shift). Part (b), the initial conditions $C_{\frac{1}{2}}(0) = \frac{1}{\sqrt{2}}e^{i\pi/2 + 0.2}$ and $C_{-\frac{1}{2}}(0) = \frac{1}{\sqrt{2}}$ (equal probabilities initially with $\frac{\pi}{2} + 0.2$ as the initial phase shift). Part (c), the initial condition $C_{\frac{1}{2}}(0)$ and $C_{-\frac{1}{2}}(0)$ have equal probabilities, and both have a random phase shift. Part (d), the initial condition $C_{\frac{1}{2}}(0) = 1$ and
$C_{-\frac{1}{2}}(0) = 0$. Since the phase shift does not affect a single initial excited state cases, part (d) does not contain any phase shift value.

The parts (a) and (d) lead near resonance to $\bar{P}_{\frac{1}{2}}(\omega/\omega_{n,e0}) \geq \bar{P}_{-\frac{1}{2}}(\omega/\omega_{n,e0})$. The part (b) and part (c) lead near resonance to $\bar{P}_{\frac{1}{2}}(\omega/\omega_{n,e0}) \leq \bar{P}_{-\frac{1}{2}}(\omega/\omega_{n,e0})$. For all cases, $\bar{P}_{\frac{1}{2}}(\omega/\omega_{n,e0}) = \bar{P}_{-\frac{1}{2}}(\omega/\omega_{n,e0})$, at resonance $\omega = \omega_{n,e0}$. In addition, the figure 4.5 also represents the $J = \frac{1}{2}$ case for $D_{\frac{1}{2}}$ and $D_{-\frac{1}{2}}$ which are identical to $C_{\frac{1}{2}}$ and $C_{-\frac{1}{2}}$ respectively.

Figure 4.6: Spin $I = 1/2$ and $0.99 \leq \frac{\omega}{\omega_{n,e0}} \leq 1.01$
In Figure 4.6, the plots of \( \bar{p}_m \) represent the average probability of \( I = \frac{1}{2} \) over the oscillation period at frequencies \( 0.99 \leq \frac{\omega}{\omega_{n0}} \leq 1.01 \). The initial conditions are identical to those presented in Figure 4.5. Parts (a), (b), and (c) demonstrate a pronounced shift at \( \frac{\omega}{\omega_{n0}} = 1 \). Moreover, in all segments, \( \bar{p}_{\frac{1}{2}} (\omega/\omega_{n0}) \) for the spin states \( \frac{1}{2} \) and \( -\frac{1}{2} \) do not intersect for \( I = \frac{1}{2} \) scenarios, except exactly at \( \omega/\omega_{n0} = 1 \), but the curve do not cross one another.

Parts (a), (b), and (c) also exhibit a distinct shift at \( \frac{\omega}{\omega_{n0}} = 1 \). This observation is consistent across all parts, further illustrating that the spin states \( \frac{1}{2} \) and \( -\frac{1}{2} \) remain non-intersecting for \( I = \frac{1}{2} \) cases.

Based on Figures 4.5 and 4.6, if the probabilities of spin states \( \frac{1}{2} \) and \( -\frac{1}{2} \) are equally likely without an initial phase shift, or if only a single spin state has a probability of 1, then the probabilities of the two spin states will never intersect. Ultimately, the initial phase shift can also impact the average probability distributions of the spin states. Specifically, if a spin state \( m \) has an initial phase shift angle \( \theta \), the resulting probabilities for \( \theta \in (-\frac{\pi}{2}, \frac{\pi}{2}) \) and \( \theta \in (\frac{\pi}{2}, \frac{3\pi}{2}) \) will differ. However, if a single state \( m \) is initially excited, then the phase shift angle \( \theta \) will not influence the outcome of the probabilities.
Figure 4.7: Spin $I = \frac{1}{2}$ and $0.95 \leq \frac{\omega}{\omega_{n,e,0}} \leq 1.05$ The Probabilities of Spin States Crossing Each Other

For example, in figure 4.7, Part (a) initial condition $C_{\frac{1}{2}} (0) = \frac{1}{\sqrt{3}}$ and $C_{-\frac{1}{2}} (0) = \sqrt{\frac{2}{3}}$. Part (b) initial condition $C_{\frac{1}{2}} (0) = \frac{1}{2}$ and $C_{-\frac{1}{2}} (0) = \sqrt{\frac{3}{2}}$. Part (c) initial condition $C_{\frac{1}{2}} (0) = \frac{1}{\sqrt{3}} e^{-i(\frac{\pi}{2}+0.2)}$ and $C_{-\frac{1}{2}} (0) = \sqrt{\frac{2}{3}} e^{-i(\frac{\pi}{2}+0.3)}$. And part (d) initial condition $C_{\frac{1}{2}} (0) = \frac{1}{2} e^{i(\frac{\pi}{2}+0.2)}$ and $C_{-\frac{1}{2}} (0) = \frac{\sqrt{3}}{2} e^{i(\frac{\pi}{2}+0.3)}$. Regardless of the phase shift for spin $I = 1/2$ or $J = 1/2$ case, the probability of each state will not cross each other within a period, if the initial states do not have equal probability or a single state dominates the probability initially.
In figure 4.8, the part (a) initial condition $C_{1/2} = \frac{1}{\sqrt{3}} e^{i(\frac{\pi}{2} + 0.2)}$ and $C_{-1/2} = \sqrt{\frac{2}{3}} e^{i(\frac{\pi}{2} + 0.3)}$. The part (b) initial condition $C_{1/2} = \frac{1}{2} e^{i(\frac{\pi}{2} + 0.2)}$ and $C_{-1/2} = \frac{\sqrt{3}}{2} e^{i(\frac{\pi}{2} + 0.3)}$. The part (c) initial condition, $C_{1/2} = \frac{1}{\sqrt{3}} e^{-i(\frac{\pi}{2} + 0.2)}$ and $C_{-1/2} = \sqrt{\frac{2}{3}} e^{-i(\frac{\pi}{2} + 0.3)}$. The part (d) initial condition, $C_{1/2} = \frac{1}{2} e^{-i(\frac{\pi}{2} + 0.2)}$ and $C_{-1/2} = \frac{\sqrt{3}}{2} e^{-i(\frac{\pi}{2} + 0.3)}$. Based on observations, switching both phase shift signs of the initial states does not affect the period averaged probabilities of each states for the $I = 1/2$ case. For example $C_{1/2} (0) = \frac{1}{2} e^{ia}$ and $C_{-1/2} (0) = \frac{\sqrt{3}}{2} e^{ib}$ the probabilities distribution will be identical to $C_{1/2} (0) = \frac{1}{2} e^{-ia}$ and $C_{-1/2} (0) = \frac{\sqrt{3}}{2} e^{-ib}$ for any arbitrary real number $a$ and $b$. 

Figure 4.8: Spin $I = \frac{1}{2}$ and $0.95 \leq \frac{\omega}{\omega_{n,e}} \leq 1.05$ Phase Affect ($\pm$)
In figure 4.9 plots of $\bar{P}_m$ the period averaged probability of $I = 1$ for frequencies satisfying $0.95 \leq \frac{\omega}{\omega_{n,e}0} \leq 1.05$. In each part, $m = 1$: (dotted black), $m = 0$: (dotted red), and $m = -1$: (solid blue). In parts (a), (b), (c) have all states initially have equal probabilities. In part (a) $C_1(0) = C_0(0) = C_{-1}(0)$, part (b) $C_1(0) e^{i(\frac{\pi}{2} + 0.2)} = C_0(0) = C_{-1}(0) = \frac{1}{\sqrt{3}}$, part (c) each state
with an initial random phase shift, part (d) $C_1 = 1$ and $C_0 = C_{-1} = 0$ only the top state was excited initially. In parts (a), (b), and (c) can find the probabilities of state 1 and $-1$ equal to each other at $\frac{\omega}{\omega_{n,e0}} = 1$ regardless of the initial phase shift of any states. In part (d), the figure will not change if any states have a phase shift initially.

Figure 4.10: Spin $I = 1$ and $0.99 \leq \frac{\omega}{\omega_{n,e0}} \leq 1.01$
As figure 4.9 and 4.10 showed, there is a sharp change of probability when \( \frac{\omega}{\omega_{n,e}} \) is close to 1 in parts (a), (b), and (c) for \( C_1 \) and \( C_{-1} \). And the probability of each state will be smooth near to \( \frac{\omega}{\omega_{n,e}} = 1 \) as a single state was excited initially as shown in part (d).

In figure 4.11, The \( \bar{P}_{\frac{3}{2}} \) (dotted black), the \( \bar{P}_{\frac{1}{2}} \) (dotted red), the \( \bar{P}_{-\frac{1}{2}} \) (solid blue), the \( \bar{P}_{-\frac{3}{2}} \) (dotted blue) as shown. \( \bar{P}_{\frac{3}{2}} = \bar{P}_{\frac{1}{2}} = \bar{P}_{-\frac{1}{2}} = \bar{P}_{-\frac{3}{2}} \) at \( \frac{\omega}{\omega_{n,e}} = 1 \). The part (a) initial conditions are \( C_{\frac{3}{2}} (0) = C_{\frac{1}{2}} (0) = C_{-\frac{1}{2}} (0) = C_{-\frac{3}{2}} = \frac{1}{2} \). The part (b) initial conditions are \( C_{\frac{3}{2}} (0) = \frac{1}{2} e^{i(\frac{\pi}{2}+0.1)} \).

Figure 4.11: Spin \( I = 3/2 \) and \( 0.95 \leq \frac{\omega}{\omega_{n,e}} \leq 1.05 \)
and $C_{\frac{1}{2}}(0) = C_{-\frac{1}{2}} = C_{-\frac{3}{2}} = \frac{1}{2}$. The part (c) initial conditions are that each state has an equal probability but a random phase shift. The part (d) initial conditions are that $C_{\frac{3}{2}}(0) = 1$ and $C_{\frac{1}{2}}(0) = C_{-\frac{1}{2}}(0) = C_{-\frac{3}{2}}(0) = 0$.

Based on figures 4.5 to 4.11, The $C_c = C_{-c}$ at $\frac{\omega}{\omega_{n,e}} = 1$ for any arbitrary spin value $c$. The average probability over a period is symmetrical about $\frac{\omega}{\omega_{n,e}} = 1$. In addition, the average probability distribution over a period is also symmetrical about the initial phase angle $\theta = 0$. For example in the $I = 1$ case, the probabilities distribution of $\bar{P}_1(t)$, $\bar{P}_0(t)$, and $\bar{P}_{-1}(0)$ will remain unchanged if initial conditions $C_1(0) = a_1 e^{i\theta_1}$, $C_0(0) = a_0 e^{i\theta_0}$, $C_{-1}(0) = a_{-1} e^{i\theta_{-1}}$ are changed to $C_1(0) = a e^{-i\theta_1}$, $C_0(0) = a_0 e^{-i\theta_0}$, $C_{-1}(0) = a_{-1} e^{-i\theta_{-1}}$, for any numbers $a_1$, $a_0$, and $a_{-1}$ satisfy $a_1^2 + a_0^2 + a_{-1}^2 = 1$. The remaining computational graphs can be found in Appendix G.

The Calculation Comparison with Gottfried’s Equation

The section is dedicated to analyzing the distinctions between Gottfried’s Solution and this research solution in this dissertation. The primary contrast between Gottfried’s solution and the proposed approach lies in the rotations that follow the clockwise rotation along the $\hat{z}$ axis.

For distinguishing the rotational angle $\beta$ from Gottfried and the present research, $\beta_G$ will represent Gottfried’s second rotational angle $\beta$, $\beta_R$ will represent the $\beta$ angle content within the present research.

Therefore, Gottfried’s $\beta_G$ can be written as

$$\sin \left( \frac{\beta_G}{2} \right) = \frac{\omega_{n1}}{\Omega_n} \sin \left( \frac{\Omega_n t}{2} \right) \quad (4.2)$$

This can be rewritten as

$$\beta_G = 2 \arcsin \left[ \frac{\omega_{n1}}{\Omega_n} \sin \left( \frac{\Omega_n t}{2} \right) \right] \quad (4.3)$$

64
And the present research’s $\beta_R$ can be written as

$$\beta_R = \arcsin \left( \frac{\omega_{n1}}{\Omega_n} \right) \quad (4.4)$$

where $\omega_{n1}$ is the frequency of the oscillating magnetic field, and $\Omega_n = \sqrt{(\omega - \omega_{n0})^2 + \omega_1^2}$ for both equations 4.3 and 4.4.

After the first clockwise rotation about the $\hat{z}$ axis, the present research produce rotate into with the fixed angle $\beta_R$ about the $\hat{y}$ axis, followed by a rotation with a constant angular velocity $\Omega_n$ about the $\hat{z}$ axis (The particular rotation is from the original angular momentum), at the last rotated back to along $\hat{y}$ axis with fixed angle $\beta_R$ again. The whole process follows the principle of conservation of angular momentum.

After the first clockwise rotation about the $\hat{z}$ axis, Gottfried made a rotation with an Euler angle $\beta_G$ about the axis $\hat{n}$, where $\hat{n} = \hat{u}_z \cos (\varphi) + \hat{u}_y \sin (\varphi)$ and $\tan \varphi = \frac{\omega_{n1}}{\omega - \omega_{n0}}$.

Then $\varphi$ can be written as

$$\varphi = \arctan \left( \frac{\omega_{n1}}{\omega - \omega_{n0}} \right) \quad (4.5)$$

Therefore, the $\hat{n}$ axis is fixed within the reference frame.

Now, there is a requirement to examine the angle $\beta_G$. Based on equation 4.3, $\beta_G$ cannot be a fixed angle, since the function of $\beta_G$ contains the time $t$.

The first time derivative of $\beta_G$ can be written as

$$\frac{\partial \beta_G}{\partial t} = \frac{\omega_{n1} \cos \frac{\Omega_n t}{2}}{\sqrt{1 - \left( \frac{\omega_{n1}}{\Omega_n} \sin \left( \frac{\Omega_n t}{2} \right) \right)^2}} \quad (4.6)$$

The rotational angle $\beta_G$ cannot satisfy the conservation of angular momentum, since the moment of inertia is a function of $r$, where $r$ is the distance from any point mass to the center of mass in the classical case.
Fig. 4.12 shows that the function \( \frac{\partial \beta_G}{\partial t} \) is not a constant angular velocity for \( \omega_{n1} = 10 \) and \( \Omega_n = 11 \), since the graph is not a linear function of \( t \).

Interestingly, for the any spin case, Gottfried’s probabilities are only work for the case of a single spin \( m \) state to a single spin \( m' \). But Gottfried’s solution is no longer consistent with the present research numerical results when the spin states are either entangled or the mixed. Since Gottfried’s rotational angle violates the law of angular momentum conservation, it won’t be accurate for any calculation that has phase shifts or spin entanglements. The related Computational code can be found in APPENDIX C.

At below, Fig. 4.13 represents the present research results for probabilities vs. time graph for spin
$I = 1/2$ case. And Fig. 4.14 represents Gottfried’s results for probabilities vs. time graphs for the spin $I = 1/2$ case.

![Graphs showing probabilities vs. time for spin $I = 1/2$](image)

**Figure 4.13:** The Computational Result for RWA Theory Spin $I = \frac{1}{2}$ Result

In Fig. 4.13, every part in the graph have the initial condition $\omega_0 = 100$ and $\omega_1 = 1$. Parts (a), (c), and (e) have the $m = 1/2$ state with an initial phase shift $e^{\frac{i\pi}{4}}$. Parts (b), (d), and (f) have no initial phase shifts. Parts (a) and (b) have the initial condition $\omega = 95$. Parts (c) and (d) have the initial condition $\omega = 99$. Parts (e) and (f) have the initial condition $\omega = 100$ (at resonance).
In Fig. 4.14, every part in the graph has the initial condition $\omega_0 = 100$ and $\omega_1 = 1$. Parts (a), (c), and (e) have the $m = 1/2$ state with an initial phase shift $e^{i\pi/4}$. Parts (b), (d), and (f) have no initial phase shifts. Parts (a) and (b) with the initial condition $\omega = 95$. Parts (c) and (d) with the initial
condition $\omega = 99$. Parts (e) and (f) with the initial condition $\omega = 100$ (at resonance).

Below, Figure 4.15 below the present research results for the probabilities vs. time graph for the spin $I = 1$ case. And figure 4.16 represents Gottfried’s results for probabilities vs. time graphs for spin $I = 1$ case. Figure 4.15 and Figure 4.16 both at the identical condition for $\omega_{n0}$, $\omega_{n1}$, and $\omega$ for 1 period of time.
In Fig. 4.15, each part in the graph has the initial conditions $\omega_0 = 100$ and $\omega_1 = 1$. Parts (a), (c), and (e) have the $m = 1$ state with an initial phase shift $e^{\frac{i\pi}{4}}$. Parts (b), (d), and (f) have no initial phase shift. Parts (a) and (b) with the initial condition $\omega = 95$. Parts (c) and (d) with the initial condition $\omega = 99$. Parts (e) and (f) with the initial condition $\omega = 100$ (at resonance).
In Fig. 4.16, each part of the graph has the initial conditions $\omega_0 = 100$ and $\omega_1 = 1$. Parts (a), (c), and (e) have the $m = 1$ state with an initial phase shift $e^{\frac{im\pi}{2}}$. Parts (b), (d), and (f) have no initial phase shifts. Parts (a) and (b) have the initial condition $\omega = 95$. Parts (c) and (d) have the initial
condition $\omega = 99$. Parts (e) and (f) have the initial condition $\omega = 100$ (at resonance).

$^{14}_7\text{N}$ Atomic Magnetic Dipole and Electric Quadrupole Moment

$^{14}_7\text{N}$, a prevalent element in all DNA and RNA molecules in nature, plays a crucial role in biochemical processes. Exploring the atomic magnetic dipole and electric quadrupole moments of the $^{14}_7\text{N}$ atom is essential for developing more accurate models for future nucleic amino acid studies, enhancing our understanding of molecular biology and genetics.

The $^{14}_7\text{N}$ atom, characterized by a nuclear spin $I = 1$, exhibits electronic spin states $J = 1/2, 3/2,$ and $5/2$ as easily found from Hund’s rules. This section details the calculations for both the magnetic dipole moment and the electric quadrupole moment corresponding to each of these $J$ values.

$^{14}_7\text{N} \text{ Atom when } I = 1, J = 1/2$

First major step is finding the $\bar{M}$ matrix for $I = 1$ and $J = 1/2$ is based on equation 3.122 and the matrix $E1_n \otimes 1_e$.

For the $I = 1$ case,

\[
I_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad I_x = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 \end{pmatrix}, \\
I_y = \begin{pmatrix} 0 & -\frac{i}{\sqrt{2}} & 0 \\ \frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} \\ 0 & \frac{i}{\sqrt{2}} & 0 \end{pmatrix}
\]

(4.7)
For the $J = 1/2$ case,

$$
J_z = \begin{pmatrix}
\frac{1}{2} & 0 \\
0 & -\frac{1}{2}
\end{pmatrix}, \quad J_x = \begin{pmatrix}
0 & \frac{1}{2} \\
\frac{1}{2} & 0
\end{pmatrix}, \quad J_y = \begin{pmatrix}
0 & -\frac{i}{2} \\
\frac{i}{2} & 0
\end{pmatrix}
$$

(4.8)

Therefore, the $K_0 \delta_{m',m} \delta_{\bar{m}',\bar{m}}$ term can be written for $J = 1/2$ and $I = 1$ as,

$$
K_0 \delta_{m',m} \delta_{\bar{m}',\bar{m}} = \begin{pmatrix}
K_0 & 0 & 0 & 0 & 0 & 0 \\
0 & K_0 & 0 & 0 & 0 & 0 \\
0 & 0 & K_0 & 0 & 0 & 0 \\
0 & 0 & 0 & K_0 & 0 & 0 \\
0 & 0 & 0 & 0 & K_0 & 0 \\
0 & 0 & 0 & 0 & 0 & K_0
\end{pmatrix}
$$

(4.9)

Then, the $K_1$ terms in Eqn. (3.122) maybe written for $J = \frac{1}{2}$ and $I = 1$ as,

$$
K_1 \left[ \delta_{m',m} \delta_{\bar{m}',\bar{m}} m\bar{m} + \frac{1}{2} \left( \delta_{m',m-1} \delta_{\bar{m}',\bar{m}} + \delta_{m',m+1} \delta_{\bar{m}',\bar{m}} + \delta_{m',m} \delta_{\bar{m}',\bar{m}+1} + \delta_{m',m} \delta_{\bar{m}',\bar{m}-1} \alpha^I_{m,+} \right) \right]
$$

$$
= \begin{pmatrix}
\frac{K_1}{2} & 0 & 0 & 0 & 0 & 0 \\
0 & -\frac{K_1}{2} & \frac{K_1}{\sqrt{2}} & 0 & 0 & 0 \\
0 & \frac{K_1}{\sqrt{2}} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{K_1}{\sqrt{2}} & 0 & 0 \\
0 & 0 & 0 & \frac{K_1}{\sqrt{2}} & -\frac{K_1}{2} & 0 \\
0 & 0 & 0 & 0 & \frac{K_1}{2} & 0
\end{pmatrix}
$$

(4.10)

$\alpha^I_{m,\pm}$ and $\alpha^J_{m,\pm}$ can be solved by equations 3.120 and 3.121.

Then, the $K_2$ terms for $I = 1$ and $J = \frac{1}{2}$ are
\[ K_2 \left\{ \delta_{m',m} \delta_{\bar{m}',\bar{m}} \left[ \bar{m} \bar{m} \left( \bar{m} \bar{m} - \frac{1}{2} \right) + \frac{1}{2} \left[ I (I + 1) - m^2 \right] \left[ J (J + 1) - \bar{m}^2 \right] \right] \\
+ \frac{1}{2} \left( \delta_{m',m-1} \delta_{\bar{m}',\bar{m}+1} \alpha_{m,-}^{I} \alpha_{m,+}^{J} \left[ 2m \bar{m} + m - \bar{m} - 1 \right] \right) \\
+ \delta_{m',m+1} \delta_{\bar{m}',\bar{m}-1} \alpha_{m,+}^{I} \alpha_{m,-}^{J} \left[ 2m \bar{m} + \bar{m} - m - 1 \right] \right) \\
+ \frac{1}{4} \left( \delta_{m',m-2} \delta_{\bar{m}',\bar{m}+2} \alpha_{m,-}^{I} \alpha_{m,+}^{J} + \delta_{m',m+2} \delta_{\bar{m}',\bar{m}-2} \alpha_{m,+}^{I} \alpha_{m,-}^{J} \right) \right\} 
\]

(4.11)

\[
\begin{pmatrix}
\frac{K_2}{4} & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{3K_2}{4} & - \frac{K_2}{2\sqrt{2}} & 0 & 0 & 0 \\
0 & - \frac{K_2}{2\sqrt{2}} & \frac{K_2}{2} & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{K_2}{2} & - \frac{K_2}{2\sqrt{2}} & 0 \\
0 & 0 & 0 & - \frac{K_2}{2\sqrt{2}} & \frac{3K_2}{4} & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{K_2}{4}
\end{pmatrix}
\]

Therefore, the \( \bar{M} \) matrix can be written as

\[
\bar{M} = 
\begin{pmatrix}
K_0 + \frac{K_1}{4} + \frac{K_2}{4} & 0 & 0 & 0 & 0 & 0 \\
0 & K_0 + \frac{K_1}{4} + \frac{3K_2}{4} & \frac{K_2}{4} & 0 & 0 & 0 \\
0 & \frac{K_2}{4} & K_0 + \frac{K_1}{4} + \frac{K_2}{4} & 0 & 0 & 0 \\
0 & 0 & 0 & K_0 + \frac{K_1}{4} + \frac{K_2}{4} & 0 & 0 \\
0 & 0 & 0 & 0 & K_0 + \frac{K_1}{4} + \frac{3K_2}{4} & 0 \\
0 & 0 & 0 & 0 & 0 & K_0 + \frac{K_1}{4} + \frac{3K_2}{4}
\end{pmatrix}
\]

(4.12)

Next \( E \mathbf{1}_n \otimes \mathbf{1}_e \) can be written as

\[
E \mathbf{1}_n \otimes \mathbf{1}_e
= 
\begin{pmatrix}
\Omega_I + \frac{1}{2} \Omega_J & 0 & 0 & 0 & 0 & 0 \\
0 & \Omega_I - \frac{1}{2} \Omega_J & 0 & 0 & 0 & 0 \\
0 & 0 & \frac{1}{2} \Omega_J & 0 & 0 & 0 \\
0 & 0 & 0 & - \frac{1}{2} \Omega_J & 0 & 0 \\
0 & 0 & 0 & 0 & - \Omega_I + \frac{1}{2} \Omega_J & 0 \\
0 & 0 & 0 & 0 & 0 & - \Omega_I - \frac{1}{2} \Omega_J
\end{pmatrix}
\]

(4.13)

The second step is set up and solve \( \det (\bar{H}_0 + \bar{M} - E \mathbf{1}_n \otimes \mathbf{1}_e) \)
Letting

\[\mu_1 = K_0 + \frac{K_1}{2} + \frac{K_2}{4}, \quad \mu_2 = K_0 - \frac{K_1}{2} + \frac{3K_2}{4}, \quad \mu_3 = K_0 + \frac{K_2}{2}, \quad \Gamma = \frac{K_1}{\sqrt{2}} - \frac{K_2}{2\sqrt{2}}\]

\[\Omega_{1,\frac{1}{2}}^{\frac{1}{2}} = \Omega_I + \frac{1}{2}\Omega_J, \quad \Omega_{1,-\frac{1}{2}}^{\frac{1}{2}} = \Omega_I - \frac{1}{2}\Omega_J, \quad \Omega_{0,\frac{1}{2}}^{\frac{1}{2}} = \frac{1}{2}\Omega_J, \quad (4.14)\]

\[\Omega_{0,-\frac{1}{2}}^{\frac{1}{2}} = -\frac{1}{2}\Omega_J, \quad \Omega_{0,\frac{1}{2}}^{\frac{1}{2}} = -\Omega_I + \frac{1}{2}\Omega_J, \quad \Omega_{-1,\frac{1}{2}}^{\frac{1}{2}} = -\Omega_I - \frac{1}{2}\Omega_J, \quad (4.14)\]

Then \(\bar{H}_0 + \bar{M} - E1_n \otimes 1_e\) can be written as

\[
\begin{pmatrix}
\mu_1 + \Omega_{1,\frac{1}{2}}^{\frac{1}{2}} & 0 & 0 & 0 & 0 & 0 \\
0 & \mu_2 + \Omega_{1,-\frac{1}{2}}^{\frac{1}{2}} & \Gamma & 0 & 0 & 0 \\
0 & \Gamma & \mu_3 + \Omega_{0,\frac{1}{2}}^{\frac{1}{2}} & 0 & 0 & 0 \\
0 & 0 & 0 & \mu_3 + \Omega_{0,-\frac{1}{2}}^{\frac{1}{2}} & \Gamma & 0 \\
0 & 0 & 0 & \Gamma & \mu_2 + \Omega_{1,-\frac{1}{2}}^{\frac{1}{2}} & 0 \\
0 & 0 & 0 & 0 & \Gamma & \mu_1 + \Omega_{1,-\frac{1}{2}}^{\frac{1}{2}}
\end{pmatrix}
\]

(4.15)

Therefore, \(\det(\bar{H}_0 + \bar{M} - E1_n \otimes 1_e)\) can be written as

\[
\det(\bar{H}_0 + \bar{M} - E1_n \otimes 1_e) \Rightarrow \left(\mu_1 + \Omega_{1,\frac{1}{2}}^{\frac{1}{2}} - \lambda\right) \left(\mu_1 + \Omega_{1,-\frac{1}{2}}^{\frac{1}{2}} - \lambda\right) \left(\mu_2 + \Omega_{1,\frac{1}{2}}^{\frac{1}{2}} - \lambda\right) \left(\mu_3 + \Omega_{0,\frac{1}{2}}^{\frac{1}{2}} - \lambda\right) - \Gamma^2\]

(4.16)

\[\times \left(\left(\mu_3 + \Omega_{0,\frac{1}{2}}^{\frac{1}{2}} - \lambda\right) \left(\mu_2 + \Omega_{1,\frac{1}{2}}^{\frac{1}{2}} - \lambda\right) - \Gamma^2\right) = 0\]

For \(\left(\mu_1 + \Omega_{1,\frac{1}{2}}^{\frac{1}{2}} - \lambda\right) \left(\mu_1 + \Omega_{1,-\frac{1}{2}}^{\frac{1}{2}} - \lambda\right)\) term can find

\[\lambda_{1,6} = K_0 + K_1/2 + K_2/4 \pm \hbar \Omega_I + \frac{1}{2}\Omega_J\]

(4.17)

Next, \(\left(\mu_2 + \Omega_{1,\frac{1}{2}}^{\frac{1}{2}} - \lambda\right) \left(\mu_3 + \Omega_{0,\frac{1}{2}}^{\frac{1}{2}} - \lambda\right) - \Gamma^2\) = 0 can be written as
\[
\left[ (\mu_2 + \Omega_{1, -\frac{1}{2}}^{\frac{1}{2}} - \lambda) \left( \mu_3 + \Omega_{0, \frac{1}{2}}^{\frac{1}{2}} - \lambda \right) - \Gamma^2 \right]
\]
\[
= \mu_2 \left( \mu_3 + \Omega_{0, \frac{1}{2}}^{\frac{1}{2}} - \lambda \right) + \Omega_{1, -\frac{1}{2}}^{\frac{1}{2}} \left( \mu_3 + \Omega_{0, \frac{1}{2}}^{\frac{1}{2}} - \lambda \right) - \lambda \left( \mu_3 + \Omega_{0, \frac{1}{2}}^{\frac{1}{2}} - \lambda \right) - \Gamma^2
\]
\[
= \mu_2 \mu_3 + \mu_2 \Omega_{0, \frac{1}{2}}^{\frac{1}{2}} - \mu_2 \lambda + \Omega_{1, -\frac{1}{2}}^{\frac{1}{2}} \mu_3 + \Omega_{1, -\frac{1}{2}}^{\frac{1}{2}} \Omega_{0, \frac{1}{2}}^{\frac{1}{2}} - \Omega_{1, -\frac{1}{2}}^{\frac{1}{2}} \lambda - \lambda \mu_3 - \lambda \Omega_{0, \frac{1}{2}}^{\frac{1}{2}} + \lambda^2 - \Gamma^2
\]
\[
= \lambda^2 - \lambda \left( \mu_2 + \mu_3 + \Omega_{1, -\frac{1}{2}}^{\frac{1}{2}} + \Omega_{0, \frac{1}{2}}^{\frac{1}{2}} \right) + \mu_2 \mu_3 + \mu_2 \Omega_{0, \frac{1}{2}}^{\frac{1}{2}} + \mu_3 \Omega_{1, -\frac{1}{2}}^{\frac{1}{2}} + \Omega_{0, \frac{1}{2}}^{\frac{1}{2}} - \Gamma^2
\]

Therefore,

\[
\lambda_{2,3} = -\frac{1}{2} \left( \mu_2 + \mu_3 + \Omega_{1, -\frac{1}{2}}^{\frac{1}{2}} + \Omega_{0, \frac{1}{2}}^{\frac{1}{2}} \right)
\]
\[
\pm \frac{1}{2} \sqrt{\left( \mu_2 + \mu_3 + \Omega_{1, -\frac{1}{2}}^{\frac{1}{2}} + \Omega_{0, \frac{1}{2}}^{\frac{1}{2}} \right)^2 - 4 \left( \mu_2 \mu_3 + \mu_2 \Omega_{0, \frac{1}{2}}^{\frac{1}{2}} + \mu_3 \Omega_{1, -\frac{1}{2}}^{\frac{1}{2}} + \Omega_{0, \frac{1}{2}}^{\frac{1}{2}} - \Gamma^2 \right)}
\]

Similarly, for \( \left[ (\mu_3 + \Omega_{0, -\frac{1}{2}}^{\frac{1}{2}} - \lambda) \left( \mu_2 + \Omega_{1, \frac{1}{2}}^{\frac{1}{2}} - \lambda \right) - \Gamma^2 \right] = 0 \) can find

\[
\lambda_{4,5} = -\frac{1}{2} \left( \mu_2 + \mu_3 + \Omega_{1, \frac{1}{2}}^{\frac{1}{2}} + \Omega_{0, -\frac{1}{2}}^{\frac{1}{2}} \right)
\]
\[
\pm \frac{1}{2} \sqrt{\left( \mu_2 + \mu_3 + \Omega_{1, \frac{1}{2}}^{\frac{1}{2}} + \Omega_{0, -\frac{1}{2}}^{\frac{1}{2}} \right)^2 - 4 \left( \mu_2 \mu_3 + \mu_2 \Omega_{0, -\frac{1}{2}}^{\frac{1}{2}} + \mu_3 \Omega_{1, \frac{1}{2}}^{\frac{1}{2}} + \Omega_{0, -\frac{1}{2}}^{\frac{1}{2}} - \Gamma^2 \right)}
\]

The corresponding computation program can be found in APPENDIX D. The numerical graph presented below is derived from the computational code, under the condition that \( K_0 : K_1 : K_2 : \omega_{p0} : \omega_{p1} : \omega_{e0} : \omega_{e1} = 1 : 1 : 2 : 100 : 1 : 1000 : 100000 \), with \( \omega \) ranging from 0 to 200000.
Figure 4.17: The Computational Result for Spin $I = 1$ and $J = \frac{1}{2}$ Result with $\omega$ Ranging from 0 to 200000

The conditions depicted in Fig. 4.17 rely solely on hypothetical assumptions for $K_0 : K_1 : K_2 : \omega_n^0 : \omega_{n1} : \omega_e^0 : \omega_{e1}$, thus failing to accurately reflect real values in the case of $^{14}_7N$.

$^{14}_7N$ Atom when $I = 1$ and $J = 3/2$

The steps for calculating $I = 1$ and $J = 3/2$ are similar to these for the $I = 1$ and $J = 1/2$ case by using equation 3.122. Similarly, assuming

\[
\begin{align*}
\mu_1 &= K_0 + \frac{3}{2}K_1 + \frac{9}{4}K_2, & \mu_2 &= K_0 + \frac{1}{2}K_1 + \frac{7}{4}K_2, & \mu_3 &= K_0 - \frac{1}{2}K_1 + \frac{9}{4}K_2, \\
\mu_4 &= K_0 - \frac{3}{2}K_1 + \frac{15}{4}K_2, & \mu_5 &= K_0 + \frac{3}{2}K_2, & \mu_6 &= K_0 + \frac{7}{2}K_2, \\
\end{align*}
\]

(4.21)
However, due to the size of the matrix, it is necessary to continue assuming

\[ A_1 = \mu_1 + \Omega_{1\frac{3}{2}} - \lambda, \quad A_2 = \mu_2 + \Omega_{1\frac{3}{2}} - \lambda, \ldots, \quad A_{12} = \mu_1 + \Omega_{-1\frac{3}{2}} - \lambda \]

for the matrix reduction process. The detailed matrix reduction process can be found in APPENDIX I. Therefore, the 12 eigenvalues of the rank 12 matrix can be written as

\[ \lambda_{1,12} = K_0 + \frac{3}{2} K_1 + \frac{9}{4} K_2 \pm \Omega_l \pm \frac{3}{2} \Omega_J \]

\[ \lambda_{2,5} = \frac{\left( \mu_2 + \mu_5 + \Omega_{1\frac{3}{2}} + \Omega_{0\frac{3}{2}} \right)}{2} \pm \sqrt{\left( \mu_2 + \mu_5 + \Omega_{1\frac{3}{2}} + \Omega_{0\frac{3}{2}} \right)^2 - 4 \left( \mu_2 \mu_5 + \mu_2 \Omega_{0\frac{3}{2}} + \mu_5 \Omega_{1\frac{3}{2}} \right)} \]

\[ \lambda_{8,11} = \frac{\left( \mu_5 + \mu_2 + \Omega_{-1\frac{3}{2}} + \Omega_{0\frac{3}{2}} \right)}{2} \pm \sqrt{\left( \mu_5 + \mu_2 + \Omega_{-1\frac{3}{2}} + \Omega_{0\frac{3}{2}} \right)^2 - 4 \left( \mu_5 \mu_2 + \mu_5 \Omega_{0\frac{3}{2}} + \mu_2 \Omega_{-1\frac{3}{2}} \right)} \]
here are list the indices for \( \lambda \) as \( m = 6, 7 \) and \( n = 1, 2 \) respectively. For example, \( \lambda_{0} \) depends upon \( X_{1}, Y_{1}, \) and \( Z_{1} \).

\[
\lambda_{m} = \frac{\sqrt[3]{2X_{n}^{3} + 3\sqrt{3}X_{n}Z - X_{n}^{2}Y_{n}^{2} + 18X_{n}Y_{n}Z_{n} - 4Y_{n}^{3} + 27Z_{n}^{2}} + 9X_{n}Y_{n} + 27Z_{n}}{\sqrt[3]{2} (-X_{n}^{2} - 3Y_{n})}
\]

\[
= \frac{\sqrt[3]{2X_{n}^{3} + 3\sqrt{3}X_{n}Z - X_{n}^{2}Y_{n}^{2} + 18X_{n}Y_{n}Z_{n} - 4Y_{n}^{3} + 27Z_{n}^{2}} + 9X_{n}Y_{n} + 27Z_{n} + \frac{X_{n}}{3}}{3}
\]

(4.27)

Similarly, list the indices of \( \lambda \) as \( m = (3, 9), (4, 10) \). For example, \( (3, 9) \) is a set of indices, representing the \( \pm \) case in the solution. Then \( n = 1, 2 \) representing the index of set of solutions. For example, \( \lambda_{3,9} \) depends upon \( X_{1}, Y_{1}, \) and \( Z_{1} \).

\[
\lambda_{m} = -\frac{1}{6\sqrt{2}} \left( 1 \pm i\sqrt{3} \right)
\]

\[
+\sqrt[3]{2X_{n}^{3} + 3\sqrt{3}X_{n}Z - X_{n}^{2}Y_{n}^{2} + 18X_{n}Y_{n}Z_{n} - 4Y_{n}^{3} + 27Z_{n}^{2}} + 9X_{n}Y_{n} + 27Z_{n}
\]

\[
+ \frac{1}{3} \times 2\frac{2}{3} \left( 2X_{n}^{3} + 3\sqrt{3}X_{n}Z - X_{n}^{2}Y_{n}^{2} + 18X_{n}Y_{n}Z_{n} - 4Y_{n}^{3} + 27Z_{n}^{2}} + 9X_{n}Y_{n} + 27Z_{n} \right)^{\frac{1}{3}}
\]

\[
+ \frac{X_{n}}{3}
\]

(4.28)

Overall, \( \lambda_{3,6,9} \) depend upon \( X_{1}, Y_{1}, \) and \( Z_{1} \), and \( \lambda_{4,7,10} \) depend upon \( X_{2}, Y_{2}, \) and \( Z_{2} \). The value for \( X_{1}, X_{2}, Y_{1}, Y_{2}, Z_{1}, \) and \( Z_{2} \) can be found in equations I.11, I.12, and I.13 in APPENDIX I.

The corresponding computation program can be found in APPENDIX D. The numerical graph presented below is derived from the computational code, under the condition that \( K_{0} : K_{1} : K_{2} \) : \( \omega_{n0} : \omega_{n1} : \omega_{e0} : \omega_{e1} = 1 : 1 : 2 : 100 : 1 : 1000 : 100000, \) with \( \omega \) ranging from 0 to 200000.
The conditions depicted in Fig. 4.18 rely solely on hypothetical assumptions for $K_0 : K_1 : K_2 : \omega_{n0} : \omega_{n1} : \omega_{e0} : \omega_{e1}$, thus failing to accurately reflect real values in the case of $^{14}_7\text{N}$.

Based on multiple tests conducted with computational code, no imaginary terms were identified in the energy levels. However, the analytical solutions provided by Eqn. (4.27) and Eqn. (4.28) suggest the potential presence of imaginary terms under certain conditions. Further investigations are required to determine the conditions that yield real values, as well as to understand the conditions under which imaginary terms might be possible, and if so, what is their consequences might be.
\[ 14 \,_7N \text{ Atom when } I = 1 \text{ and } J = 5/2 \]

The steps for calculating the \( I = 1 \) and \( J = 5/2 \) states are also similar to these for \( I = 1 \) and \( J = 1/2 \) case by using Eqn. (3.122). Similarly, assuming

\[
\begin{align*}
\mu_1 &= K_0 + \frac{5}{2} K_1 + \frac{25}{4} K_2, \\
\mu_2 &= K_0 + \frac{3}{2} K_1 + \frac{19}{4} K_2, \\
\mu_3 &= K_0 + \frac{1}{2} K_1 + \frac{17}{4} K_2, \\
\mu_4 &= K_0 - \frac{1}{2} K_1 + \frac{19}{4} K_2, \\
\mu_5 &= K_0 - \frac{3}{2} K_1 + \frac{25}{4} K_2, \\
\mu_6 &= K_0 - \frac{5}{2} K_1 + \frac{35}{4} K_2, \\
\mu_7 &= K_0 + \frac{5}{2} K_2, \\
\mu_8 &= K_0 + \frac{13}{2} K_2, \\
\mu_9 &= K_0 + \frac{17}{2} K_2
\end{align*}
\] (4.29)

\[
\begin{align*}
\Omega_{1, \frac{3}{2}} &= \Omega_I + \frac{5}{2} \Omega_J, \\
\Omega_{1, \frac{3}{2}} &= \Omega_I + \frac{3}{2} \Omega_J, \\
\Omega_{1, -\frac{1}{2}} &= \Omega_I - \frac{5}{2} \Omega_J, \\
\Omega_{1, -\frac{1}{2}} &= \Omega_I - \frac{3}{2} \Omega_J, \\
\Omega_{0, \frac{3}{2}} &= \Omega_I - \frac{1}{2} \Omega_J, \\
\Omega_{0, -\frac{1}{2}} &= \Omega_I - \frac{3}{2} \Omega_J, \\
\Omega_{0, -\frac{3}{2}} &= \Omega_I - \frac{5}{2} \Omega_J, \\
\Omega_{0, -\frac{5}{2}} &= \Omega_I - \frac{3}{2} \Omega_J
\end{align*}
\] (4.30)

\[
\begin{align*}
\Gamma_1 &= \frac{1}{2} \sqrt{\frac{5}{2}} (2K_1 + 3K_2), \\
\Gamma_2 &= 2K_1 + K_2, \\
\Gamma_3 &= \frac{3(2K_1 - K_2)}{2\sqrt{2}}, \\
\Gamma_4 &= 2K_1 - 3K_2, \\
\Gamma_5 &= \frac{1}{2} \sqrt{\frac{5}{2}} (2K_1 - 5K_2)
\end{align*}
\] (4.31)

\[
\delta_1 = \sqrt{10} K_2, \quad \delta_2 = 3\sqrt{2} K_2
\] (4.32)

Similarly, due to the size of the rank 18 matrix, it is necessary to continue assuming

\[
\begin{align*}
A_1 &= \mu_1 + \Omega_{1, \frac{3}{2}} - \lambda, \\
A_2 &= \mu_2 + \Omega_{1, \frac{3}{2}} - \lambda, \\
\cdots \\
A_{18} &= \mu_1 + \Omega_{-1, -\frac{3}{2}} - \lambda
\end{align*}
\] (4.33)
for the matrix reduction process. (The detailed matrix reduction process can be found in Appendix I)

\[ \lambda_{1,18} = \mu_1 + \Omega_{\pm 1, \pm \frac{3}{2}}^{\frac{1}{2}} \]  
\[ \lambda_{2,7} = \frac{\left( \mu_2 + \mu_7 + \Omega_{\pm 1, \pm \frac{3}{2}}^{\frac{1}{2}} + \Omega_{\pm 1, \pm \frac{3}{2}}^{\frac{1}{2}} \right)}{2} \]

\[ \pm \sqrt{\left( \mu_2 + \mu_7 + \Omega_{\pm 1, \pm \frac{3}{2}}^{\frac{1}{2}} + \Omega_{\pm 1, \pm \frac{3}{2}}^{\frac{1}{2}} \right)^2 - 4 \left( \mu_2 \mu_7 + \mu_2 \Omega_{\pm 1, \pm \frac{3}{2}}^{\frac{1}{2}} + \mu_7 \Omega_{\pm 1, \pm \frac{3}{2}}^{\frac{1}{2}} + \Omega_{\pm 1, \pm \frac{3}{2}}^{\frac{1}{2}} \Omega_{\pm 1, \pm \frac{3}{2}}^{\frac{1}{2}} \right)} \]

\[ \left| \begin{array}{cc} A_{12} & \Gamma_1 \\ \Gamma_1 & A_{17} \end{array} \right| = A_{12} A_{17} - \Gamma_1^2 = \left( \mu_7 + \Omega_{0, \pm \frac{3}{2}}^{\frac{1}{2}} - \lambda \right) \left( \mu_2 + \Omega_{-1, \pm \frac{3}{2}}^{\frac{1}{2}} - \lambda \right) - \Gamma_1^2 \]

\[ = \lambda^2 - \lambda \left( \mu_2 + \mu_7 + \Omega_{-1, \pm \frac{3}{2}}^{\frac{1}{2}} + \Omega_{0, \pm \frac{3}{2}}^{\frac{1}{2}} \right) \]

\[ + \mu_2 \mu_7 + \mu_2 \Omega_{0, \pm \frac{3}{2}}^{\frac{1}{2}} + \mu_7 \Omega_{-1, \pm \frac{3}{2}}^{\frac{1}{2}} + \Omega_{0, \pm \frac{3}{2}}^{\frac{1}{2}} \Omega_{-1, \pm \frac{3}{2}}^{\frac{1}{2}} \]

List the indices of \( \lambda \) as \( m = 9, 8, 5, 6 \) and \( n = 3, 4, 5, 6 \) respectively. For example, \( \lambda_9 \) depends upon \( X_3, Y_3, \) and \( Z_3 \). Therefore, the solution of \( \lambda \) can be written as

\[ \lambda_m = \frac{\sqrt{2} X_n^3 + 3 \sqrt{3} \sqrt{4 X_n^3 Z_n - X_n^2 Y_n^2 + 18 X_n Y_n Z_n - 4 Y_n^3 + 27 Z_n^2 + 9 X_n Y_n + 27 Z_n}}{3 \sqrt{2}} \]

\[ - \frac{\sqrt{2} (-X_n^2 - 3 Y_n)}{3 \sqrt{3} X_n^3 + 3 \sqrt{3} \sqrt{4 X_n^3 Z_n - X_n^2 Y_n^2 + 18 X_n Y_n Z_n - 4 Y_n^3 + 27 Z_n^2 + 9 X_n Y_n + 27 Z_n}} \]

\[ + \frac{X_n}{3} \]

(4.37)

Similarly, list the indices of \( \lambda \) as \( m = (4, 14), (3, 13), (10, 15), (11, 16) \). For example, \( (4, 14) \) is a set of indices, representing the \( \pm \) cases in the solution. Then \( n = 3, 4, 5, 6 \) representing the indices
of set of solutions. For example, \( \lambda_{4,14} \) contain \( X_3, Y_3, Z_3 \).

\[
\lambda_m = -\frac{1}{6\sqrt{2}} \left( 1 \pm i\sqrt{3} \right) \\
+ \sqrt[3]{2X_n^3 + 3\sqrt{3} \left( 4X_n^3Z_n - X_n^2Y_n^2 + 18X_nY_nZ_n - 4Y_n^3 + 27Z_n^2 + 9X_nY_n + 27Z_n \right)} \\
+ \frac{X_n}{3} \\
+ \left( 1 \mp i\sqrt{3} \right) (-X_n^2 - 3Y_n) \\
\times 2^{\frac{2}{3}} \left( 2X_n^3 + 3\sqrt{3} \left( 4X_n^3Z_n - X_n^2Y_n^2 + 18X_nY_nZ_n - 4Y_n^3 + 27Z_n^2 + 9X_nY_n + 27Z_n \right) \right)^{\frac{1}{3}}
\]

(4.38)

In here, \( \lambda_{4,9,14} \) contain \( X_3, Y_3, \) and \( Z_3 \); \( \lambda_{3,8,13} \) contain \( X_4, Y_4, \) and \( Z_4 \); \( \lambda_{10,5,15} \) contain \( X_5, Y_5, \) and \( Z_5 \); and \( \lambda_{11,6,16} \) contain \( X_6, Y_6, \) and \( Z_6 \). \( X_3, X_4, X_5, X_6, Y_3, Y_4, Y_5, Y_6, Z_3, Z_4, Z_5, \) and \( Z_6 \) can be found in equations I.29, I.31, I.33, and I.35 in APPENDIX I.

The corresponding computation program can be found in APPENDIX D. The numerical graph presented below is derived from computational code, under the condition that \( K_0 : K_1 : K_2 : \omega_{n0} : \omega_{n1} : \omega_{e0} : \omega_{e1} = 1 : 1 : 2 : 100 : 1 : 1000 : 100000 \), with \( \omega \) ranging from 0 to 200000.
Figure 4.19: The Computational Result for Spin $I = 1$ and $J = \frac{5}{2}$ Result with $\omega$ Ranging from 0 to 200000

The conditions depicted in Fig. 4.19 rely solely on hypothetical assumptions for $K_0 : K_1 : K_2 : \omega_n : \omega_{n1} : \omega_e : \omega_{e1}$, thus failing to accurately reflect real values in the case of $^{14}N$.

Based on multiple tests conducted with computational code, no imaginary terms were identified in the energy levels. However, the analytical solutions provided by Eqn. (4.37) and Eqn. (4.38) suggest the potential presence of imaginary terms under certain conditions. Further investigations are required to determine the conditions that yield real values, as well as to understand the conditions under which imaginary terms appear, and if so, what their physical consequences might be.
Among all isotopes, $\text{Li}$ has the lowest requirement for a magnetic octupole moment, with a nuclear spin of $I = 3/2$ and an electronic total angular momentum of $J = 1/2$, so the combined matrix for the energies has rank 8. Additionally, lithium is a crucial element for batteries and electricity storage. Understanding the electric quadrupole and magnetic octupole moments of the $\text{Li}$ atom could potentially aid in building more accurate models for simulations and modeling.

Similar to $^{14}\text{N}$ calculation, $\text{Li}$ needs to simplify $\tilde{H}_0 + \tilde{M} - E 1_n \otimes 1_e$ by assuming

$$
\begin{align*}
\mu_1 &= K_0 + \frac{3}{4} K_1 + \frac{9}{16} K_2 + \frac{27}{64} K_3, \\
\mu_2 &= K_0 - \frac{3}{4} K_1 + \frac{21}{16} K_2 - \frac{87}{64} K_3 \\
\mu_3 &= K_0 + \frac{1}{6} K_1 + \frac{13}{16} K_2 - \frac{11}{64} K_3, \\
\mu_4 &= K_0 - \frac{1}{4} K_1 + \frac{17}{16} K_2 - \frac{49}{64} K_3
\end{align*}
$$

(4.39)

$$
\begin{align*}
\Omega_{\frac{3}{2},\frac{3}{2}}^{\frac{1}{2},\frac{1}{2}} &= \frac{3}{2} \Omega_I + \frac{1}{2} \Omega_J, \\
\Omega_{\frac{3}{2},-\frac{3}{2}}^{\frac{3}{2},\frac{3}{2}} &= \frac{3}{2} \Omega_I - \frac{1}{2} \Omega_J, \\
\Omega_{\frac{3}{2},-\frac{3}{2}}^{\frac{1}{2},-\frac{1}{2}} &= \frac{1}{2} \Omega_I + \frac{1}{2} \Omega_J, \\
\Omega_{\frac{3}{2},-\frac{3}{2}}^{\frac{1}{2},-\frac{1}{2}} &= -\frac{1}{2} \Omega_I - \frac{1}{2} \Omega_J
\end{align*}
$$

(4.40)

$$
\Gamma_1 = \frac{\sqrt{3}}{32} \left(16K_1 - 8K_2 + 19K_3\right), \quad \Gamma_2 = K_1 - \frac{1}{2} K_2 + \frac{19}{16} K_3
$$

(4.41)

Continue defining,

$$
\begin{align*}
A_1 &= \mu_1 + \Omega_{\frac{3}{2},\frac{3}{2}}^{\frac{1}{2},\frac{1}{2}} - \lambda, \\
A_2 &= \mu_2 + \Omega_{\frac{3}{2},-\frac{3}{2}}^{\frac{3}{2},\frac{3}{2}} - \lambda, \\
A_3 &= \mu_3 + \Omega_{\frac{3}{2},\frac{3}{2}}^{\frac{1}{2},\frac{1}{2}} - \lambda, \\
A_4 &= \mu_4 + \Omega_{\frac{3}{2},-\frac{3}{2}}^{\frac{3}{2},\frac{3}{2}} - \lambda, \\
A_5 &= \mu_4 + \Omega_{\frac{3}{2},-\frac{3}{2}}^{\frac{3}{2},\frac{3}{2}} - \lambda, \\
A_6 &= \mu_3 + \Omega_{\frac{3}{2},\frac{3}{2}}^{\frac{1}{2},\frac{1}{2}} - \lambda
\end{align*}
$$

(4.42)

$$
\begin{align*}
A_7 &= \mu_2 + \Omega_{\frac{3}{2},\frac{3}{2}}^{\frac{1}{2},-\frac{1}{2}} - \lambda, \\
A_8 &= \mu_1 + \Omega_{\frac{3}{2},\frac{3}{2}}^{\frac{1}{2},-\frac{1}{2}} - \lambda
\end{align*}
$$
Therefore, \( \det (\hat{H}_0 + \tilde{M} - E1_n \otimes 1_e - 1\lambda) \) can be written as

\[
\begin{pmatrix}
A_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & A_2 & \Gamma_1 & 0 & 0 & 0 & 0 & 0 \\
0 & \Gamma_1 & A_3 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & A_4 & \Gamma_2 & 0 & 0 & 0 \\
0 & 0 & 0 & \Gamma_2 & A_5 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & A_6 & \Gamma_1 & 0 \\
0 & 0 & 0 & 0 & \Gamma_1 & A_7 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & A_8
\end{pmatrix}
\]

(4.43)

Which reduce to 2 matrices of rank 1 and 3 matrices of rank 2, then can find

\[
\lambda_{1,8} = \mu_1 + \Omega_{\frac{3}{2},\frac{3}{2},\pm\frac{1}{2}}
\]

(4.44)

then the eigenvalues of the 3 rank 2 matrices’ eigenvalues are

\[
\lambda_{2,3} = \frac{\left( \mu_2 + \mu_3 + \Omega_{\frac{3}{2},\frac{3}{2},\frac{1}{2}} + \Omega_{\frac{3}{2},\frac{3}{2},\frac{1}{2}} \right)}{2}
\]

\[
\pm \sqrt{\left( \mu_2 + \mu_3 + \Omega_{\frac{3}{2},\frac{3}{2},\frac{1}{2}} + \Omega_{\frac{3}{2},\frac{3}{2},\frac{1}{2}} \right)^2 - 4 \left( \mu_2 \mu_3 + \mu_2 \Omega_{\frac{3}{2},\frac{3}{2},\frac{1}{2}} + \mu_3 \Omega_{\frac{3}{2},\frac{3}{2},\frac{1}{2}} + \Omega_{\frac{3}{2},\frac{3}{2},\frac{1}{2}} - \Gamma_2 \right)}}\]

(4.45)

\[
\lambda_{4,5} = \frac{\left( 2\mu_4 + \Omega_{\frac{3}{2},\frac{3}{2},\frac{3}{2}} + \Omega_{\frac{3}{2},\frac{3}{2},\frac{3}{2}} \right)}{2}
\]

\[
\pm \sqrt{\left( 2\mu_4 + \Omega_{\frac{3}{2},\frac{3}{2},\frac{3}{2}} + \Omega_{\frac{3}{2},\frac{3}{2},\frac{3}{2}} \right)^2 - 4 \left( \mu_4^2 + \mu_4 \left( \Omega_{\frac{3}{2},\frac{3}{2},\frac{3}{2}} + \Omega_{\frac{3}{2},\frac{3}{2},\frac{3}{2}} \right) + \Omega_{\frac{3}{2},\frac{3}{2},\frac{3}{2}} \Omega_{\frac{3}{2},\frac{3}{2},\frac{3}{2}} - \Gamma_4 \right)}}\]

(4.46)
\[
\lambda_{6,7} = \frac{\left( \mu_2 + \mu_3 + \Omega_{\frac{3}{2}, \frac{1}{2}} + \Omega_{\frac{3}{2}, -\frac{1}{2}} \right)}{2} \\
\pm \sqrt{\left( \mu_2 + \mu_3 + \Omega_{\frac{3}{2}, \frac{1}{2}} + \Omega_{\frac{3}{2}, -\frac{1}{2}} \right)^2 - 4 \left( \mu_2 \mu_3 + \mu_2 \Omega_{\frac{3}{2}, \frac{1}{2}} + \mu_3 \Omega_{\frac{3}{2}, \frac{1}{2}} + \Omega_{\frac{3}{2}, -\frac{1}{2}} \Omega_{\frac{3}{2}, -\frac{1}{2}} - \Gamma_1^2 \right)}
\]

(4.47)

The corresponding computation program can be found in APPENDIX D. The numerical graph presented below is derived from computational code, under the condition that \( K_0 : K_1 : K_2 : K_3 : \omega_{n0} : \omega_{n1} : \omega_{e0} : \omega_{e1} = 1 : 1 : 2 : 4 : 100 : 1 : 1000 : 100000 \), with \( \omega \) ranging from 0 to 200000.

Figure 4.20: The Computational Result for Spin \( I = \frac{3}{2} \) and \( J = \frac{1}{2} \) Result with \( \omega \) Ranging from 0 to 200000
The conditions depicted in Fig. 4.20 rely solely on the hypothetical assumptions for $K_0 : K_1 : K_2 : K_3 : \omega_{n0} : \omega_{n1} : \omega_{e0} : \omega_{e1}$, thus failing to accurately reflect real values in the case of $^7_3\text{Li}$.

**Lie Algebra Extension**

Derived from the rotation analysis conducted in the present research, the concept can be extended to a general Lie algebra framework. Initially, an arbitrary set of 3D Lie groups $\{O_\mu\} = \{X, Y, Z\}$ is considered. In accordance with the definition of a Lie group, the set $\{X, Y, Z\}$ must satisfy the following criteria,

$$[O_\mu, O_\nu] = \kappa \epsilon_{\mu\nu\lambda} O_\lambda$$  \hspace{1cm} (4.48)

where $\kappa$ is some coefficient of the given Lie group, and $\epsilon_{\mu\nu\lambda}$ is the Levi-Civita symbol.

Based on the Jacobi identity $[O_\mu, O_\mu] = 0$,

$$[X, [Y, Z]] + [Y, [Z, X]] + [Z, [X, Y]] = 0$$ \hspace{1cm} (4.49)

where $X$, $Y$, and $Z$ are three linear independent vectors [65].

Therefore, for any arbitrary 3D Lie Group $\{O_\mu\} = \{X, Y, Z\}$, if $X$, $Y$, and $Z$ are linear independent variables, for any function $f (X, Y) = aX + bY$ can be transformed to

$$e^{f(X,Y)} = e^{aX+bY} = e^{\gamma Z} e^{-\alpha X} e^{-\gamma Z}$$ \hspace{1cm} (4.50)

where $a$ and $b$ are the random coefficients in front of $X$ and $Y$. The $\gamma$ and $\alpha$ are the corresponding coefficients which can satisfy the relation.

To establish the validity of this relationship, the Eqn. (4.50) can be rearranged initially.

$$e^{-\gamma Z} e^{aX+bY} e^{\gamma Z} = e^{-\alpha X}$$ \hspace{1cm} (4.51)
The right side Eqn. (4.51) can be written as
\[ e^{-\alpha X} = \sum_{k=0}^{\infty} \frac{(-\alpha X)^k}{k!} \quad (4.52) \]

The left side Eqn. (4.51) can be written as
\[ e^{-\gamma Z} e^{aX + bY} e^{\gamma Z} = e^{-\gamma Z} \left[ \sum_{k=0}^{\infty} \frac{(aX + bY)^k}{k!} \right] e^{\gamma Z} \quad (4.53) \]

Subsequently, the condition for
\[ \sum_{k=0}^{\infty} e^{-\gamma Z} \left[ \frac{(aX + bY)^k}{k!} \right] e^{\gamma Z} = \sum_{k=0}^{\infty} \frac{(-\alpha X)^k}{k!} \quad (4.54) \]

The random single term in the summation on the left in Eqn. (4.54), can be written as
\[ e^{-\gamma Z} \left[ \frac{(aX + bY)^k}{k!} \right] e^{\gamma Z} = \frac{1}{k!} e^{-\gamma Z} (aX + bY) e^{\gamma Z} \quad (4.55) \]

Then for each \( e^{-\gamma Z} (aX + bY) e^{\gamma Z} \) term can be written as
\[ e^{-\gamma Z} (aX + bY) e^{\gamma Z} = ae^{-\gamma Z} X e^{\gamma Z} + be^{-\gamma Z} Y e^{\gamma Z} \quad (4.56) \]

The first derivative of \( e^{-\gamma Z} X e^{\gamma Z} \) can be written as,
\[ \frac{d}{d\gamma} \left( e^{-\gamma Z} X e^{\gamma Z} \right) = -\kappa e^{-\gamma Z} Y e^{\gamma Z} \quad (4.57) \]

The first derivative of \( e^{-\gamma Z} Y e^{\gamma Z} \) can be written as,
\[ \frac{d}{d\gamma} \left( e^{-\gamma Z} Y e^{\gamma Z} \right) = \kappa e^{-\gamma Z} X e^{\gamma Z} \quad (4.58) \]
Drawing upon the first-order differential Eqns (4.57) and (4.58), it is reasonable to assume

\[ e^{-\gamma Z}Xe^{\gamma Z} = A \sin (\kappa \gamma) + B \cos (\kappa \gamma) \]  

(4.59)

Then, based on Eqn. (4.57), \( e^{-\gamma Z}Ye^{\gamma Z} \) can be written as

\[ e^{-\gamma Z}Ye^{\gamma Z} = -A \cos (\kappa \gamma) + B \sin (\kappa \gamma) \]  

(4.60)

Based on the boundary condition when \( \gamma \to 0 \), Eqn. (4.59) can be expressed as,

\[ \lim_{\gamma \to 0} e^{-\gamma Z}Xe^{\gamma Z} = A \sin (0) + B \cos (0) = B = X \]  

(4.61)

Similarly, Eqn. (4.60) can be shown as,

\[ \lim_{\gamma \to 0} e^{-\gamma Z}Ye^{\gamma Z} = -A \cos (0) + B \sin (0) = -A = Y \]  

(4.62)

Therefore, Eqn. (4.59) can be rewritten as,

\[ e^{-\gamma Z}Xe^{\gamma Z} = -Y \sin (\kappa \gamma) + X \cos (\kappa \gamma) \]  

(4.63)

And, Eqn. (4.60) can be written as

\[ e^{-\gamma Z}Ye^{\gamma Z} = Y \cos (\kappa \gamma) + X \sin (\kappa \gamma) \]  

(4.64)

Subsequently, Eqn. (4.63) and Equation (4.64) can be substituted into Equation (4.56).

\[ e^{-\gamma Z}(aX + bY)e^{\gamma Z} = a [-Y \sin (\kappa \gamma) + X \cos (\kappa \gamma)] + b [Y \cos (\kappa \gamma) + X \sin (\kappa \gamma)] \]  

\[ = X [a \cos (\kappa \gamma) + b \sin (\kappa \gamma)] + Y [-a \sin (\kappa \gamma) + b \cos (\kappa \gamma)] \]  

(4.65)
Therefore, based on Eqn. (4.54), Eqn. (4.55), and Eqn. (4.65) can be written as,

\[-\alpha X = X \left[ a \cos (\kappa \gamma) + b \sin (\kappa \gamma) \right] + Y \left[ -a \sin (\kappa \gamma) + b \cos (\kappa \gamma) \right] \] (4.66)

Then based on the X terms in Eqn. (4.66) can find,

\[-\alpha = a \cos (\kappa \gamma) + b \sin (\kappa \gamma) \] (4.67)

And based on the Y terms in Eqn. (4.66) can obtain,

\[0 = -a \sin (\kappa \gamma) + b \cos (\kappa \gamma) \] (4.68)

Therefore, the relationship between \(a\), \(b\), and \(\kappa \gamma\) can be written as,

\[\frac{b}{a} = \tan \kappa \gamma \] (4.69)

Then \(\kappa \gamma\) can be written as,

\[\kappa \gamma = \arctan \left( \frac{b}{a} \right) = \arcsin \left( \frac{b}{\sqrt{a^2 + b^2}} \right) = \arccos \left( \frac{a}{\sqrt{a^2 + b^2}} \right) \] (4.70)

Additionally, one could determine,

\[\sin (\kappa \gamma) = \frac{b}{\sqrt{a^2 + b^2}}, \quad \cos (\kappa \gamma) = \frac{a}{\sqrt{a^2 + b^2}}, \quad \alpha = -\sqrt{a^2 + b^2} \] (4.71)

From the aforementioned considerations, it is evident that

\[e^{\alpha X + b Y} = e^{\arcsin \left( \frac{b}{\sqrt{a^2 + b^2}} \right) \frac{Z}{\kappa}} e^{\sqrt{a^2 + b^2} X} e^{-\arcsin \left( \frac{b}{\sqrt{a^2 + b^2}} \right) \frac{Z}{\kappa}} \] (4.72)
The rotation can readily extend to another axis and can be expressed as

\[ e^{aX + bY + cZ} = e^{\gamma Z} e^{\beta Y} e^{\theta X} e^{-\gamma Z} \]  

(4.73)

Similarly Eqn. (4.73) can be written as

\[ e^{-\beta Y} e^{-\gamma Z} e^{aX + bY + cZ} e^{\gamma Z} e^{\beta Y} = e^{\theta X} \]  

(4.74)

Then the left side can be shown as,

\[ e^{-\beta Y} e^{-\gamma Z} e^{aX + bY + cZ} e^{\gamma Z} e^{\beta Y} = e^{-\beta Y} e^{-\gamma Z} \sum_{k=0}^{\infty} \frac{(aX + bY + cZ)^k}{k!} e^{\gamma Z} e^{\beta Y} \]  

(4.75)

The right side can be shown as,

\[ e^{\theta X} = \sum_{k=0}^{\infty} \frac{\theta X)^k}{k!} \]  

(4.76)

Similar to Eqn. (4.55) case, any single term in Eqn. (4.75) also can be written as

\[ \frac{1}{k!} e^{-\beta Y} e^{-\gamma Z} (aX + bY + cZ)^k e^{\gamma Z} e^{\beta Y} \]

\[ = \frac{1}{k!} e^{-\beta Y} e^{-\gamma Z} (aX + bY + cZ) e^{\gamma Z} e^{\beta Y} e^{-\gamma Z} (aX + bY + cZ) e^{\gamma Z} e^{\beta Y} \]  

\[ \cdots e^{-\beta Y} e^{-\gamma Z} (aX + bY + cZ) e^{\gamma Z} e^{\beta Y} \]  

(4.77)

Based on Eqn. (4.72), then \( e^{-\beta Y} e^{-\gamma Z} (aX + bY + cZ) e^{\gamma Z} e^{\beta Y} \) can be written as

\[ e^{-\beta Y} e^{-\gamma Z} (aX + bY + cZ) e^{\gamma Z} e^{\beta Y} = e^{-\beta Y} \left( \sqrt{a^2 + b^2} X + cZ \right) e^{\beta Y} \]  

(4.78)

Then Eqn. (4.72) can be rewritten as,

\[ e^{-\beta Y} \left( \sqrt{a^2 + b^2} X + cZ \right) e^{\beta Y} = e^{-\beta Y} \sqrt{a^2 + b^2} X e^{\beta Y} + e^{-\beta Y} cZ e^{\beta Y} \]  

(4.79)
The first derivative of $e^{-\beta Y} \sqrt{a^2 + b^2 X} e^{\beta Y}$ can be expressed as,

$$\frac{d}{d\beta} \left( e^{-\beta Y} \sqrt{a^2 + b^2 X} e^{\beta Y} \right) = \kappa e^{-\beta Y} \sqrt{a^2 + b^2} Z e^{\beta Y}$$  \hspace{1cm} (4.80)

The first derivative of $e^{-\beta Y} Ze^{\beta Y}$ can be shown as,

$$\frac{d}{d\beta} \left( e^{-\beta Y} Ze^{\beta Y} \right) = -\kappa e^{-\beta Y} X e^{\beta Y}$$  \hspace{1cm} (4.81)

Hence, it is reasonable to assume,

$$e^{-\beta Y} X e^{\beta Y} = A \sin (\kappa \beta) + B \cos (\kappa \beta)$$  \hspace{1cm} (4.82)

Then, $e^{-\beta Y} Ze^{\beta Y}$ can be written as,

$$e^{-\beta Y} Ze^{\beta Y} = A \cos (\kappa \beta) - B \sin (\kappa \beta)$$  \hspace{1cm} (4.83)

Now, both cases can be considered alongside the boundary condition $\beta \to 0$ to determine,

$$\lim_{\beta \to 0} e^{-\beta Y} X e^{\beta Y} = X = A \sin (0) + B \cos (0) = B$$  \hspace{1cm} (4.84)

$$\lim_{\beta \to 0} e^{-\beta Y} Ze^{\beta Y} = Z = A \cos (0) - B \sin (0) = A$$  \hspace{1cm} (4.85)

Based on the coefficients above, Eqn. (4.79) can be written as

$$e^{-\beta Y} \left( \sqrt{a^2 + b^2} X + c Z \right) e^{\beta Y}$$

$$= \sqrt{a^2 + b^2} [Z \sin (\kappa \beta) + X \cos (\kappa \beta)] + c [Z \cos (\kappa \beta) - X \sin (\kappa \beta)]$$  \hspace{1cm} (4.86)

$$= Z \left[ \sqrt{a^2 + b^2} \sin (\kappa \beta) + c \cos (\kappa \beta) \right] + X \left[ \sqrt{a^2 + b^2} \cos (\kappa \beta) - c \sin (\kappa \beta) \right]$$
Henceforth, relying on Eqn. (4.74) and Eqn. (4.86), one can determine

\[
\sqrt{a^2 + b^2} \sin (\kappa \beta) + c \cos (\kappa \beta) = 0
\]  

(4.87)

Consequently, the solution can be found

\[
\kappa \beta = \arctan \left( - \frac{c}{\sqrt{a^2 + b^2}} \right) = \arcsin \left( \frac{c}{\sqrt{a^2 + b^2 + c^2}} \right) = \arccos \left( \frac{\sqrt{a^2 + b^2}}{\sqrt{a^2 + b^2 + c^2}} \right)
\]  

(4.88)

Then \( \theta \) can be written as

\[
\theta = \sqrt{a^2 + b^2} \cos (\kappa \beta) - c \sin (\kappa \beta) = \sqrt{a^2 + b^2 + c^2}
\]  

(4.89)

Therefore, it can be concluded that,

\[
e^{aX + bY + cZ} = \exp \left[ \arcsin \left( \frac{b}{\sqrt{a^2 + b^2}} \right) \frac{Z}{\kappa} \right] \exp \left[ \arcsin \left( \frac{c}{\sqrt{a^2 + b^2 + c^2}} \right) \frac{Y}{\kappa} \right] \exp \left[ \sqrt{a^2 + b^2 + c^2} X \right] \\
\times \exp \left[ - \arcsin \left( \frac{c}{\sqrt{a^2 + b^2 + c^2}} \right) \frac{Y}{\kappa} \right] \exp \left[ - \arcsin \left( \frac{b}{\sqrt{a^2 + b^2}} \right) \frac{Z}{\kappa} \right]
\]  

(4.90)

Given that rotations can commence from any axis and each rotation can proceed in either clockwise or counterclockwise directions, there exist \( 12 = 3! \cdot 2 \) distinct methods to accomplish the rotations.

NMR Test Runs for \( ^{14}_7\text{N} \) in Cytosine

The nucleus of \( ^{14}_7\text{N} \) exhibits a nuclear spin \( I = 1 \), and it can interact with electron spins \( J = 1/2, 3/2, \) and \( 5/2 \), leading to different cases of electronic quadrupole moments. This variability in \( J \)
values often results in the broadening of peaks in the NMR spectra of $^{14}_7$N, rendering them difficult to distinguish. Recent research, however, has demonstrated the feasibility of obtaining distinct $^{14}_7$N NMR peaks in 1,3,5-triaminobenzene hydrochloride by employing a solvent mixture of DMSO-d6 and acetone in a 1:3 ratio, supplemented with a small amount of HCl [35]. This breakthrough has illuminated the potential for applying $^{14}_7$N NMR spectroscopy to nucleic amino acids. The current focus lies on examining $^{14}_7$N within cytosine, a compound that presents challenges in dissolution within a DMSO-d6 and acetone solution at a 1:3 ratio when a small amount of DCl is added. However, it has been discovered that initial dissolution of cytosine in DCl, followed by the introduction of the DMSO-d6 and acetone solution, effectively overcomes these solubility issues. This methodological adjustment offers a promising avenue for facilitating the study of cytosine and potentially other amino acids through $^{14}_7$N NMR spectroscopy.

Figure 4.21: Cytosine Sample Test 14
Fig. 4.21 presents the solution NMR spectra for $^{14}{_7}$N in cytosine. The analyzed sample comprised 0.006g of cytosine, 400$\mu$L of 3.5% DC1, 100$\mu$L of DMSO-d6, and 400$\mu$L of deuterated acetone, subjected to 2048 scan repetitions.

Nevertheless, the NMR spectra of $^{14}{_7}$N in cytosine remain excessively broad, presenting considerable challenges for analysis. To address this, it was decided to adjust the solvent mixture ratios, specifically by altering the DMSO-d6 and acetone solution to 1:4, 1:5, and 1:6 ratios. This modification aims to reduce the viscosity of DMSO-d6, with the anticipation that such changes could improve the clarity and interpretability of the NMR spectra. The ultimate goal is to facilitate more detailed and accurate analyses.

Figure 4.22: Cytosine Sample Test 22

Fig. 4.22 presents the solution NMR spectra for $^{14}{_7}$N in cytosine. The analyzed sample comprised...
0.0038g of cytosine, 100µL of 4% DCl, 100µL of DMSO-d6, and 400µL of deuterated acetone, subjected to 2048 scan repetitions.

Upon comparing Figures 4.21 and 4.22, it is observed that both samples contain identical amounts of DMSO-d6 and Acetone, yet they differ in the quantity of DCl. Further analysis from additional experimental runs indicates that with cytosine quantities exceeding 0.0009g, the outcomes tend to be consistent across the board. However, the pronounced discrepancy between Figures 4.21 and 4.22 has hindered a productive analysis.

After conducting the initial test runs, a series of four experiments was initiated to explore the effects of DCl concentration and the ratios between DMSO-d6 and acetone.
Fig. 4.23 presents the solution NMR spectra for $^{14}$N in cytosine. The analyzed sample comprised 0.0045g of cytosine, 100µL of 4% DCl, 100µL of DMSO-d6, and 500µL of deuterated acetone, subjected to 8096 scan repetitions. All discernible peaks have been annotated manually.
Fig. 4.24 presents the solution NMR spectra for $^{14}$N in cytosine. The analyzed sample comprised 0.0024g of Cytosine, 50µL of 4% DCl, 100µL of DMSO-d6, and 500µL of deuterated acetone, subjected to 8192 scan repetitions. All discernible peaks have been annotated manually.
Fig. 4.25 presents the solution NMR spectra for $^{14}$N in cytosine. The analyzed sample comprised 0.0009g of Cytosine, 50µL of 4% DCl, 100µL of DMSO-d6, and 600µL of deuterated acetone, subjected to 8192 scan repetitions. All discernible peaks have been annotated manually.
Fig. 4.26 presents the solution NMR spectra for $^{14}$N in cytosine. The analyzed sample comprised 0.0014g of Cytosine, 50µL of 0.4% DCI, 20µL of 4% DCI, 100µL of DMSO-d6, and 600µL of deuterated acetone, subjected to 8192 scan repetitions. All discernible peaks have been annotated manually. In this experiment, an initial addition of 50µL of 0.4% DCI was insufficient to fully dissolve the cytosine, necessitating the subsequent incorporation of an additional 20µL of 4% DCI to achieve complete dissolution.

To facilitate easier recognition of features, a code for noise reduction was also developed.
Fig. 4.27 presents the solution NMR spectra for $^{14}$N in cytosine test 25 before noise reduction.

Fig. 4.28: Cytosine Sample Test 25 in Python After Noise Reduction
Fig. 4.28 presents the solution NMR spectra for $^{14}_7$N in cytosine test 25 after noise reduction. The code successfully eliminated most of the noise, yet it inadvertently also diminished the sharp peaks within the graph. In the context of $^{14}_7$N NMR spectra for cytosine, there are only a few sharp peaks, which can be identified by referencing the original NMR spectra. The identification of local maxima now enables the tracking of chemical shifts across the sample tests.

![Data with Local Maxima](image)

Figure 4.29: Cytosine Sample Test 25 in Python After Noise Reduction Local Maxima

Fig. 4.29 presents the solution NMR spectra for $^{14}_7$N in cytosine test 25 after noise reduction local maxima. This strategy facilitates the comparison between cytosine test 25 and cytosine test 26.
Variations in DCl concentration were observed to have minimal impact on the peaks around -39 ppm, 117.8 ppm, and 321 ppm, indicating stable chemical shifts at these frequencies. Conversely, the peaks at 864 ppm, 836 ppm, 422 ppm, and 359 ppm in Test 25 exhibited higher intensities compared to Test 26. On the other hand, Test 26 showed greater peak intensities around 604 ppm and 42 ppm than Test 25. Additionally, a notable chemical shift was detected in the range from 480 ppm to 530 ppm, further illustrating the influence of DCl concentration on the NMR spectra.

Furthermore, a comparative analysis between cytosine test 26 and cytosine test 27 can also be conducted.
Fig. 4.31 presents the solution NMR spectra for $^{14}$N in cytosine after noise reduction test 26 and test 27 with local maxima.

In the graphical representation, it is observed that the peaks around 226 ppm are closely aligned with each other. Moreover, referencing the original graphs 4.24 and 4.25, it is noted that the peak at 321 ppm also exhibits a close proximity between the two tests. Consequently, this suggests that the ratio of DMSO-d6 to Acetone exerts minimal influence on these specific peaks. In contrast, significant shifts are observed in the remainder of the peaks, with some peaks present in test 26 nearly vanishing in test 27.

To further confirm that the ratio of DMSO-d6 to acetone exerts a more pronounced effect on chemical shifts than the concentration of DCl, a comparison between test 27 and test 28 was conducted.
Fig. 4.32 presents the solution NMR spectra for $^{14}_7$N in cytosine after noise reduction test 27 and test 28 with local maxima.

Fig. 4.32 demonstrates similar behaviors to Fig. 4.30, where in some regions the peaks of test 27 are higher than those in test 28, and vice versa. However, the overall structure of tests 27 and 28 exhibits a remarkable similarity.
Fig. 4.33 presents the solution NMR spectra for $^{14}$N in Cytosine after noise reduction test 25, test 26, test 27, and test 28 with local maxima. As anticipated, tests 25 and 26 bear a resemblance to one another, as do tests 27 and 28. Nonetheless, the distinctions between the pairs of tests 25 and 26 versus tests 27 and 28 are markedly pronounced.

The current local maxima identification test requires further enhancements. Among cytosine simple tests 25 to 28, some peaks were not successfully recognized by the algorithm. Additionally, there is a misalignment between some peaks and their corresponding local maxima, suggesting the necessity for integrating an improved algorithm in subsequent versions.
Schwinger’s 1937 paper adeptly calculated the coefficients of each spin state for the frequency range opposite to that containing the Larmor frequency. Although his approach was unconventional in quantum mechanics and did not account for the resonance within its range, it is significant that Schwinger’s work is often overlooked in citations (Schwinger, 1937) [12]. Gottfried’s equation aligns with the results for transitions between individual spin states \( m \) and \( m' \) (Gottfried, 1966)[14]. However, Gottfried’s second rotation appears to violate the law of conservation of angular momentum, leading to inaccuracies in describing spin states with initial phase shifts or in entangled states.

Unfortunately, most research up to today has used Gottfried’s second rotation \( \beta_G \) result for NMR simulations, which could potentially yield inaccurate results. In addition, the standard NMR Hamiltonian cannot be solved numerically using perturbation theory, since the perturbation has to be done to infinite order. However, the research that we have conducted has precisely solved for the general nuclear spin state function appropriate for NMR. The rotating wave approach was initially employed to allow the reference frame to rotate along with the oscillating magnetic field. Subsequently, the spin state system was treated analogously to a Rubik’s Cube, applying similar techniques to diagonalize the time-dependent parts of the state function.

The general electron spin state function appropriate for EPR can be derived using the same methodology, which has opened the door for two new potential experiments that connect NMR and EPR together for both atoms and molecules. Thus, the exact forms of both nuclear and electron spin state functions were utilized to construct a doubly-rotated ground state for time-dependent
perturbation calculations. Given that the Hamiltonians for the magnetic dipole moment, the electron quadrupole moment, and the magnetic octupole moment all include terms that are powers of \( I \cdot J \), the sub-state energy levels for the perturbations were also calculated. These differ from the standard hyperfine electronic structure that only considers the electron spin energy levels. We also used this method to calculate the sub-state energy levels for \(^{14}\)N and \(^{7}\)Li.

Secondly, the state function that we derived can be used for the calculations of quantum state entanglements and potentially for developments in quantum information and quantum gate theories. The precise dynamics of our state functions show their potential for their use in atoms with nuclear spins larger than \( \frac{1}{2} \), which could enhance development in quantum computing.

From the derivation of the general nuclear spin state function, the approach was expanded to include the general Lie group for 3D rotations along three linearly independent axes. We transformed each operator matrix exponential such as \( e^{aX} \), \( e^{bY} \), and \( e^{cZ} \) into harmonic oscillators. Therefore, any two operators with linearly combined terms such as the exponential of \( f(X, Y) = aX + bY \), which can also be written as three exponentials of single matrices multiplied with each other. Our research method can also separate the combined linear function such as an exponential of \( f(X, Y, Z) = aX + bY + cZ \) into products of five exponentials of single matrices, with each term containing only one operator \( X \), \( Y \), or \( Z \). It was discovered that there are a total of 12 different methods to accomplish rotations in any arbitrary direction using these three axes.

The current focus is on producing NMR spectra for \(^{14}\)N in nucleic amino acids.
Future Studies

There remain several interactions and rotational scenarios within molecules that require consideration. Additionally, the lattice structure of the sample must be taken into account in future calculations. Subsequently, it may be possible to construct a simulation encompassing multiple molecules within solution and solid sample systems by applying our novel quantum state function to the method of Rabi, Ramsey, and Schwinger in 1954 [13].

For $^{133}_{55}$Cs, the ground state is $I = \frac{7}{2}, J = \frac{1}{2}$. Recent experiments have been in disagreement about its electric quadrupole and magnetic octupole moments. We propose that our new method to measure the energy levels that combines the NMR and EPR experiments to obtain these and allowing for the first accurate measurement of all seven of the nuclear moments for that isotope, including the hexadecapole and higher moments contained in the Hamiltonian $H = \sum_{n=0}^{7} (I \cdot J)^{n} K_{n}$.

The generalized spin state functions of nuclei in NMR and electrons in EPR can also be extended to the realm of quantum entanglement, potentially leading to the development of improved theoretical frameworks for quantum computing. This advancement could open up new avenues for establishing quantum gates, and precise calculations of quantum entanglement.
APPENDIX A: COMPUTATIONAL CODE FOR NUCLEAR AND ELECTRON SPINS
Presented below is the computer code designed for automatically computing the probabilities of various nuclear spin (or electronic spin) configurations in NMR.

```mathematica
Print["Let's make sure all varibles are cleared at the first"]; ClearAll[t, n, \[Omega], \[Tau], Ostate, K, i, Fstate]; Print["All Clear"]; TN = 0.008(* TN is for Thickness of the plot, the usual value range \ is between 0.001 to 0.008. *)
TN1 = 0.05(* TN1 is for Thickness of the legend line in the plot *)
n = 1;(*n is the nuclear spin number*)
Ostate = {{0}, {1}, {0}}; (* Ostate is the normalized initial state \ of the nuclear spin, it has to be normalized*)
Fstate = {{0}, {0}, {0}}; (* Fstate is the normalized final state of the nuclear spin which you are interested for calculating the \ probability, it has to be normalized. However, you can make all as 0, \ if you want to see the calculation and plot for all possibile states \ probability changes through 1 period *)
If[ ConjugateTranspose[Ostate] . Ostate != {{1}},
   Print["Please check the initial state, it is not normalized!"];
   Abort[];
```

112
If ConjugateTranspose[Fstate] . Fstate != {{1}} &&
ConjugateTranspose[Fstate] . Fstate != {{0}},
Print["Please check the final state, it is not normalized!"];
Abort[];
]
If[Length[Ostate] == Length[Fstate] == 2*n + 1 &&
ConjugateTranspose[Fstate] . Fstate == {{0}},
If [ConjugateTranspose[Ostate] . Ostate == {{1}},
If[Length[Ostate] == 2*n + 1,
i = 1;
ID = IdentityMatrix[2*n + 1];
Iz = ID;
Ix = ID;
Iy = ID;
IzE = ID;
Print[ID // MatrixForm];
For [i = 1, i < 2*n + 2, i++, Iz[[i, i]] = (n - i + 1)];
For [i = 1, i < 2*n + 2, i++,
IzE[[i, i]] = (n - i + 1)*
Sqrt[(Subscript[\Omega, 0] - \Omega)^2 + Subscript[\Omega, 1]^2];
Print["Iz matrix for spin ", n, " is "];
Print[Iz // MatrixForm];
Print["The energy level matrix for ", n, " Spin is "];

For[i = 1, i < 2*n + 2, i++]
Ix[[i + 1, i]] = Sqrt[(2*n - i + 1)*i]/2;

For [i = 1, i < 2*n + 2, i++,
Ix[[i, i + 1]] = Sqrt[(2*n - i + 1)*i]/2];

For [i = 1, i < 2*n + 2, i++,
Ix[[i, i]] = 0];

Print["Ix matrix for spin ", n, " is "];
Print[Ix // MatrixForm];

For [i = 1, i < 2*n + 2, i++,
Iy[[i + 1, i]] = I*Sqrt[(2*n - i + 1)*i]/2];

For [i = 1, i < 2*n + 2, i++,
Iy[[i, i + 1]] = -I*Sqrt[(2*n - i + 1)*i]/2];

For [i = 1, i < 2*n + 2, i++,
Iy[[i, i]] = 0];

Print["Iy matrix for spin ", n, " is "];
Print[Iy // MatrixForm];

Beta =
ArcSin[Subscript[\[Omega], 1]/
Sqrt[(Subscript[\[Omega], 0] - \[Omega])^2 + Subscript[\[Omega], 1]^2]]; 

IyT = MatrixExp[-I*Iy*Beta];

IyTT = MatrixExp[I*Iy*Beta];

Print["The transformation matrix for Iy is "];
Print[IyT // MatrixForm];

Print["The transformation matrix for Iz is "];
\[
\text{IzT} = \text{MatrixExp}[-\text{I} \cdot \text{Iz} \cdot [\Omega] \cdot t];
\]
\[
\text{Print}[\text{IzT} // \text{MatrixForm}];
\]
\[
\text{Print["The transformation matrix for the Berry Phase is "]};
\]
\[
\text{IzET} = \text{MatrixExp}[-\text{I} \cdot \text{IzE} \cdot t];
\]
\[
\text{Print}[\text{IzET} // \text{MatrixForm}];
\]
\[
\text{Print["The transformation matrix for the states is "]};
\]
\[
\text{MT} = \text{Simplify}[\text{IzT} \cdot \text{IyT} \cdot \text{IzET} \cdot \text{IyTT}];
\]
\[
\text{Print}[\text{MT} // \text{MatrixForm}];
\]
\[
\text{t} = \tau \cdot 2 \cdot \pi / \sqrt{([\Omega_0]^2 + [\Omega_1]^2)};
\]
\[
\text{MT} = \text{Simplify}[\text{IzT} \cdot \text{IyT} \cdot \text{IzET} \cdot \text{IyTT}];
\]
\[
\text{Print}[\text{MT} // \text{MatrixForm}];
\]
\[
\text{State} = \text{Simplify}[\text{MT} \cdot \text{Ostate}];
\]

(* Below is the conditions of the magnetic field for plotting the final states' probabilities, you can change here for making the plot *)

[\Omega] = 99; (* [\Omega] is the angular velocity of the magnetic field on the xy plane *)

[\Omega_1] = 1; (* [\Omega_1] is the angular velocity of the magnetic field on the xy plane *)
is the oscillatory magnetic field term on the \(xy\) plane \(\ast\)

\[\text{Subscript}[\Omega, 0] = 100; \quad (* \text{Subscript}[\Omega, 0]\]

is the constant magnetic field term on the \(z\)-axis \(\ast\)

\(* \text{Above are the conditions of the magnetic field for plotting}\)

\(* \text{the final states' probabilities, you can change here for making the}\)

\(* \text{plot}\ast\)

\begin{verbatim}
K = 
Do[AppendTo[K, Part[ID, i]], {i, 1, 2n + 1}];
P = 
Do[AppendTo[P,
    SetPrecision[Conjugate[Part[State, i]]*Part[State, i], (*
        Here, we can set up the precision for the graph,
        the initial setting is at 30-digit precision,
        the maximum precision is the MachinePrecision which means
        the exact number\ast\)30(*The precision number\ast*)]], {i, 1, 2n + 1}];
PP = Plot[P, \{\[Tau], 0, 1\}, PlotLegends -> {{K}},
    PlotLegends -> Thickness[TN1], PlotStyle -> {Thickness[TN]},
    PlotRange -> Full,
    TicksStyle -> {{FontSize -> 16, Black}, {FontSize -> 16, Black}}];
Print[PP];
\end{verbatim}
If[Length[Ostate] != 2*n + 1,
    Print["Please check the spin number and the initial state!"];
    Abort[]];

If[ConjugateTranspose[Ostate] . Ostate != {{1}},
    Print["Please check the initial state, it is not normalized!"];
    Abort[];]

If[Length[Ostate] == Length[Fstate] == 2*n + 1 &&
    ConjugateTranspose[Fstate] . Fstate == {{1}} &&
    ConjugateTranspose[Ostate] . Ostate == {{1}},
    i = 1;
    ID = IdentityMatrix[2*n + 1];
    Iz = ID;
    Ix = ID;
    Iy = ID;
    IzE = ID;
    Print[ID // MatrixForm];
    For [i = 1, i < 2*n + 2, i++, Iz[[i, i]] = (n - i + 1)];
    For [i = 1, i < 2*n + 2, i++,
        IzE[[i, i]] = (n - i + 1)*
            Sqrt[(Subscript[\[Omega], 0] - \[Omega])ˆ2 + Subscript[\[Omega],
            1]ˆ2]];
    Print["Iz matrix for spin ", n, " is "];
    Print[Iz // MatrixForm];
The energy level matrix for \( n \) Spin is \\
For \( i = 1, i < 2n + 2, i++ \)
\[ Ix[[i + 1, i]] = \sqrt{(2n - i + 1)\cdot i}/2 \] \\
For \( i = 1, i < 2n + 2, i++ \)
\[ Ix[[i, i + 1]] = \sqrt{(2n - i + 1)\cdot i}/2 \] \\
For \( i = 1, i < 2n + 2, i++ \)
\[ Ix[[i, i]] = 0 \] \\
Print["Ix matrix for spin ", n, " is "]
Print[Ix // MatrixForm];
For \( i = 1, i < 2n + 2, i++ \)
\[ Iy[[i + 1, i]] = I\cdot \sqrt{(2n - i + 1)\cdot i}/2 \] \\
For \( i = 1, i < 2n + 2, i++ \)
\[ Iy[[i, i + 1]] = -I\cdot \sqrt{(2n - i + 1)\cdot i}/2 \] \\
For \( i = 1, i < 2n + 2, i++ \)
\[ Iy[[i, i]] = 0 \] \\
Print["Iy matrix for spin ", n, " is "]
Print[Iy // MatrixForm];
\[ \beta = \text{ArcSin}[\omega_1/\sqrt{(\omega_0 - \omega)^2 + \omega_1^2}] \] \\
IyT = \text{MatrixExp}[-I\cdot Iy\cdot \beta];
IyTT = \text{MatrixExp}[I\cdot Iy\cdot \beta];
Print["The transformation matrix for Iy is "];
Print[IyT // MatrixForm];
Print["The transformation matrix for Iz is "];
IzT = MatrixExp[-I*Iz*[Omega]*t];
Print[IzT // MatrixForm];
Print["The transformation matrix for the Berry Phase is "];
IzET = MatrixExp[-I*IzE*t];
Print[IzET // MatrixForm];
Print["The transformation matrix for the states is "];
MT = Simplify[IzT . IyT . IzET . IyTT];
Print[MT // MatrixForm];
t = [Tau]*2*Pi/
   Sqrt[(Subscript[\[Omega], 0] - \[Omega])^2 + Subscript[\[Omega], 1]^2];
MT = Simplify[IzT . IyT . IzET . IyTT];
Print[MT // MatrixForm];
State = Simplify[MT . Ostate];
K = {Fstate};

(* Below is the conditions of the magnetic field for plotting 
   the 
   individual final state probability, you can change here for 
   making 
   the plot*)
\[Omega] = 99;(* \[Omega] is the angular velocity of the magnetic field in 
   the 

Subscript[\[\Omega\], 1] = 1; (* Subscript[\[\Omega\], 1] is the oscillatory magnetic field term on the xy plane *)

Subscript[\[\Omega\], 0] = 100; (* Subscript[\[\Omega\], 0] is the constant magnetic field term on the z-axis *)

(* Above are the conditions of the magnetic field for plotting the individual final state probability, you can change here for making the plot *)

P = SetPrecision[
ConjugateTranspose[
    ConjugateTranspose[State] .
    Fstate] . (ConjugateTranspose[State] . Fstate), (* Here, we can set up the precision for the graph, the initial setting is at 30-digit precision, the maximum precision is the MachinePrecision which means the exact number *) 30 (*The precision number*)];
PP = Plot[P, \{\[Tau], 0, 1\}, PlotLegends -> \{\{K\}\},
  PlotLegends -> Thickness[TN1], PlotStyle -> \{Thickness[TN]\},
  PlotRange -> Full,
  TicksStyle -> \{\{FontSize -> 16, Black\}, \{FontSize -> 16, Black\}\}];
Print[PP];
]
If[Length[Ostate] != Length[Fstate],
  Print["Please check the final state, it does have the same size as \ the initial state!"];
]
If[Length[Ostate] == Length[Fstate] != 2*n + 1,
  Print["Please check the initial state, the final state, and the spin \ number, they do not have the same size!"];
]
APPENDIX B: THE TIME AVERAGES OF THE OCCUPATION PROBABILITIES
The code below is for the time averages of the occupation probabilities based on

\[ P_{m,\bar{m}} = \frac{1}{T_{n,e}} \int_0^{T_{n,e}} P_{m,\bar{m}}(t) \, dt \]  

(B.1)

```
1 Print["Let's make sure all variables are cleared at the first"];  
2 ClearAll[t, n, \[Omega], \[Tau], Ostate, K, i, Fstate];  
3 Print["All Clear"];  
4 TN = 0.008(* TN is for Thickness of the plot, the usual value  
   range \  
   is between 0.001 to 0.008. *)  
5 TN1 = 0.05(* TN1 is for Thickness of the legend line in the plot  
   *)  
6 n = 1;(*n is the nuclear spin number*)  
7 Ostate = {{1/Sqrt[3]*Exp[I*(Pi/2 + 0.1)]}, {1/Sqrt[3]}, {1/Sqrt[3]}}; (* Ostate is the normalized initial state of the  
   nuclear spin, it has to be normalized*)  
8 Fstate = {{0}, {0}, {0}}; (* Fstate is the normalized final state  
   of the  
   nuclear spin which you are interested for calculating the \  
   probability, it has to be normalized. However, you can make all  
   as 0, \  
   if you want to see calculation and plot for all possible states \  
   probability changes through 1 period *)  
9 If[ ConjugateTranspose[Ostate] . Ostate != {{1}},  
10 Print["Please check the initial state, it is not normalized!"];  
11```

123
Abort[];

If[ ConjugateTranspose[Fstate] . Fstate != {{1}} && ConjugateTranspose[Fstate] . Fstate != {{0}},
   Print["Please check the final state, it is not normalized!"]; Abort[];
]

If[Length[Ostate] == Length[Fstate] == 2*n + 1 && ConjugateTranspose[Fstate] . Fstate == {{0}},
   If[ConjugateTranspose[Ostate] . Ostate == {{1}},
      If[Length[Ostate] == 2*n + 1,
         i = 1;
         ID = IdentityMatrix[2*n + 1];
         Iz = ID;
         Ix = ID;
         Iy = ID;
         IzE = ID;
         Print[ID // MatrixForm];
         For [i = 1, i < 2*n + 2, i++, Iz[[i, i]] = (n - i + 1)];
         For [i = 1, i < 2*n + 2, i++,
            IzE[[i, i]] = (n - i + 1)*
            Sqrt[(Subscript[\[Omega], 0] - \[Omega])^2 + Subscript[\[Omega], 1]^2];
         Print["Iz matrix for spin ", n, " is "];
      ]
   ]
]
Print[Iz // MatrixForm];
Print["The energy level matrix for ", n, " Spin is "];
For[i = 1, i < 2*n + 2, i++,
   Ix[[i + 1, i]] = Sqrt[(2*n - i + 1)*i]/2;]
For[i = 1, i < 2*n + 2, i++,
   Ix[[i, i + 1]] = Sqrt[(2*n - i + 1)*i]/2;]
For[i = 1, i < 2*n + 2, i++, Ix[[i, i]] = 0];
Print["Ix matrix for spin ", n, " is "];
Print[Ix // MatrixForm];
For[i = 1, i < 2*n + 2, i++,
   Iy[[i + 1, i]] = I*Sqrt[(2*n - i + 1)*i]/2]
For[i = 1, i < 2*n + 2, i++,
   Iy[[i, i + 1]] = -I*Sqrt[(2*n - i + 1)*i]/2;]
For[i = 1, i < 2*n + 2, i++, Iy[[i, i]] = 0];
Print["Iy matrix for spin ", n, " is "];
Print[Iy // MatrixForm];
\[Beta] =
ArcSin[Subscript[\[Omega], 1]/
Sqrt[(Subscript[\[Omega], 0] - \[Omega])^2 + Subscript[\[Omega],
1]^2]];
IyT = MatrixExp[-I*Iy*\[Beta]];
IyTT = MatrixExp[I*Iy*\[Beta]];
Print["The transformation matrix for Iy is "];
Print[IyT // MatrixForm];
Print["The transformation matrix for Iz is "];
IzT = MatrixExp[-I*Iz*\[Omega]*t];
Print[IzT // MatrixForm];
Print["The transformation matrix for the Berry Phase is "];
IzET = MatrixExp[-I*IzE*t];
Print[IzET // MatrixForm];
Print["The transformation matrix for the states is "];
MT = Simplify[IzT . IyT . IzET . IyTT];
Print[MT // MatrixForm];
t = \[Tau]*2*Pi/
Sqrt[(Subscript[\[Omega], 0] - \[Omega])^2 + Subscript[\[Omega], 1]^2];
MT = Simplify[IzT . IyT . IzET . IyTT];
Print[MT // MatrixForm];
State = Simplify[MT . Ostate];

(* Below is the conditions of the magnetic field for plotting
the \final states' probabilities, you can change here for making the
plot*)
Subscript[\[Omega], 1] = 1; (* Subscript[\[Omega], 1]
is the oscillatory magnetic field term in the xy plane *)
Subscript[\[Omega], 0] = 100; (* Subscript[\[Omega], 0]
is the constant magnetic field term about the z-axis *)

\[ \Omega = a \times \text{Subscript}[\Omega, 0]; (* \[Omega] is the angular velocity of the magnetic field in the xy plane, a=[Omega]/Subscript[\Omega, 0] *)

(* Above are the conditions of the magnetic field for plotting the final states' probabilities, you can change here for making the plot*)

K = {};
Do[AppendTo[K, Part[ID, i]], {i, 1, 2*n + 1}];
P = {};
Do[AppendTo[P,
  Integrate[Refine[Conjugate[Part[State, i]]*Part[State, i], \{Element[\[Tau], Reals], Element[a, Reals]\}], \{\[Tau], 0, 1]\}], {i, 1, 2*n + 1}];
PP = Plot[
P, \{a, 0.95, 1.05(*Here, we can change the number for the range of x axis, a=[Omega]/Subscript[\Omega, 0]*)\}, PlotLegends -> {{K}},
PlotLegends -> Thickness[TN1], PlotStyle -> {Thickness[TN]},}]}
PlotRange -> Full,
TicksStyle -> {{FontSize -> 16, Black}, {FontSize -> 16, Black}}];
Print[PP];
]
If[Length[Ostate] != 2*n + 1,
Print["Please check the spin number and the initial state!"];
Abort[]];
If[ConjugateTranspose[Ostate] . Ostate != {{1}},
Print["Please check the initial state, it is not normalized!"];
Abort[]];
]
If[Length[Ostate] == Length[Fstate] == 2*n + 1 &&
ConjugateTranspose[Fstate] . Fstate == {{1}} &&
ConjugateTranspose[Ostate] . Ostate == {{1}},
i = 1;
ID = IdentityMatrix[2*n + 1];
Iz = ID;
Ix = ID;
Iy = ID;
IzE = ID;
Print[ID // MatrixForm];
For [i = 1, i < 2*n + 2, i++, Iz[[i, i]] = (n - i + 1)];
For [i = 1, i < 2*n + 2, i++,
IzE[[i, i]] = (n - i + 1)*
\[
\sqrt{(\omega_0 - \omega)^2 + \omega_1^2};
\]

Print["Iz matrix for spin ", n, " is "];
Print[Iz // MatrixForm];
Print["The energy level matrix for ", n, " Spin is "];
For[i = 1, i < 2*n + 2, i++,
Ix[[i + 1, i]] = \sqrt{(2*n - i + 1)*i}/2;
For [i = 1, i < 2*n + 2, i++,
Ix[[i, i + 1]] = \sqrt{(2*n - i + 1)*i}/2];
For [i = 1, i < 2*n + 2, i++, Ix[[i, i]] = 0];
Print["Ix matrix for spin ", n, " is "]
Print[Ix // MatrixForm];
For [i = 1, i < 2*n + 2, i++,
Iy[[i + 1, i]] = I*\sqrt{(2*n - i + 1)*i}/2]
For [i = 1, i < 2*n + 2, i++,
Iy[[i, i + 1]] = -I*\sqrt{(2*n - i + 1)*i}/2];
For [i = 1, i < 2*n + 2, i++, Iy[[i, i]] = 0];
Print["Iy matrix for spin ", n, " is "];
Print[Iy // MatrixForm];
\[\beta = \]
ArcSin[Subscript[\[Omega], 1]/
\sqrt{(Subscript[\[Omega], 0] - \[Omega])^2 + Subscript[\[Omega], 1]^2}];
IyT = MatrixExp[-I*Iy*\[Beta]\];
IyTT = MatrixExp[I*Iy*\[Beta]\];
Print["The transformation matrix for Iy is "];
Print[IyT // MatrixForm];
Print["The transformation matrix for Iz is "];
IzT = MatrixExp[-I*Iz*\[Omega]*t];
Print[IzT // MatrixForm];
Print["The transformation matrix for the Berry Phase is "];
IzET = MatrixExp[-I*IzE*t];
Print[IzET // MatrixForm];
Print["The transformation matrix for the states is "];
MT = Simplify[IzT . IyT . IzET . IyTT];
Print[MT // MatrixForm];
t = \[Tau]*2*Pi/
Sqrt[(\[Omega], 0) - \[Omega]]^2 + \[Omega],^2];
MT = Simplify[IzT . IyT . IzET . IyTT];
Print[MT // MatrixForm];
State = Simplify[MT . Ostate];
K = {Fstate};

(* Below is the conditions of the magnetic field for plotting
the \
individual final state probability, you can change here for

making
the plot*)

Subscript[\[\Omega], 1] = 1; (* Subscript[\[\Omega], 1] is the oscillatory magnetic field
term \n
on the xy plane *)

Subscript[\[\Omega], 0] = 100; (* Subscript[\[\Omega], 0] is the constant magnetic field
term \n
on the z-axis *)

\[\Omega] =
  a*Subscript[\[\Omega],
  0];(* \[\Omega] is the angular velocity of the magnetic field
  on \n  the xy plane, a=\[\Omega]/Subscript[\[\Omega], 0] *)

(* Above are the conditions of the magnetic field for plotting
  the \n  individual final state probability, you can change here for
  making \n  the plot*)

P = Integrate[
  Refine[ConjugateTranspose[
    ConjugateTranspose[State] .
```
Fstate] . (ConjugateTranspose[State] . Fstate), {Element[[\[Tau], Reals], Element[a, Reals]]}, {[
\[Tau],
0, 1]};

PP = Plot[
  P, {a, 0.95, 1.05(*Here, we can change the number for the range of x axis, a=\[Omega]/Subscript[\[Omega], 0]*)}, PlotLegends -> {{K}},
  PlotLegends -> Thickness[TN1], PlotStyle -> {Thickness[TN]},
  PlotRange -> Full,
  TicksStyle -> {{FontSize -> 16, Black}, {FontSize -> 16, Black}}];

Print[PP];

If[Length[Ostate] != Length[Fstate],
  Print["Please check the final state, it does have the same size as \the initial state!"];
]

If[Length[Ostate] == Length[Fstate] != 2*n + 1,
  Print["Please check the initial state, the final state, and the spin \number, they do not have the same size!"];
]
APPENDIX C: COMPUTATIONAL CODE TO COMPARE THE RESEARCH TRANSITION MATRICES AND GOTTFRIED’S TRANSITION MATRICES
The Research Transition Matrices

The following code has been developed specifically for research purposes concerning transition matrices. It represents a comprehensive solution meticulously crafted to compute transition matrices for arbitrary spin states.

```
Print["Let's make sure all variables are cleared at the first"]; ClearAll[t, \[Omega], Subscript[\[Omega], 0], Subscript[\[Omega], 1], n, i, \[Tau]]; Print["All Clear"]; n = 3; (*The nuclear spin I = 3*) i = 1; ID = IdentityMatrix[2*n + 1]; Iz = ID; Ix = ID; Iy = ID; IzE = ID; Print[ID // MatrixForm]; For [i = 1, i < 2*n + 2, i++, Iz[[i, i]] = (n - i + 1)]; For [i = 1, i < 2*n + 2, i++, IzE[[i, i]] = (n - i + 1)*Sqrt[(Subscript[\[Omega], 0] - \[Omega])^2 + Subscript[\[Omega], 1]^2]]; Print["Iz matrix for spin ", n, " is "];```

134
Print[Iz // MatrixForm];
Print["The energy level matrix for ", n, " Spin is "];
For[i = 1, i < 2*n + 2, i++, Ix[[i + 1, i]] = Sqrt[(2*n - i + 1)*i]/2];
For [i = 1, i < 2*n + 2, i++,
Ix[[i, i + 1]] = Sqrt[(2*n - i + 1)*i]/2];
For [i = 1, i < 2*n + 2, i++, Ix[[i, i]] = 0];
Print["Ix matrix for spin ", n, " is "];
Print[Ix // MatrixForm];
For [i = 1, i < 2*n + 2, i++,
Iy[[i + 1, i]] = I*Sqrt[(2*n - i + 1)*i]/2]
For [i = 1, i < 2*n + 2, i++, Iy[[i, i + 1]] = -I*Sqrt[(2*n - i + 1)*i]/2];
For [i = 1, i < 2*n + 2, i++, Iy[[i, i]] = 0];
Print["Iy matrix for spin ", n, " is "];
Print[Iy // MatrixForm];
\[Beta\] = ArcSin[Subscript[\[Omega], 1]/
Sqrt[(Subscript[\[Omega], 0] - \[Omega])^2 + Subscript[\[Omega], 1]^2]]; 
IyT = FullSimplify[MatrixExp[-I*Iy*\[Beta]]];
IyTT = FullSimplify[MatrixExp[I*Iy*\[Beta]]];
Print[IyT // MatrixForm];
IzET = MatrixExp[-I*IzE*t];
The Gottfried Transition Matrices

The code for Gottfried’s transitional matrices, showcased below, embodies a versatile implementation crafted to compute transitional matrices for spin numbers of any magnitude.
Iz = ID;
Ix = ID;
Iy = ID;
IzE = ID;

Print[ID // MatrixForm];
For [i = 1, i < 2*n + 2, i++, Iz[[i, i]] = (n - i + 1)];
For [i = 1, i < 2*n + 2, i++,
    IzE[[i, i]] = (n - i + 1)*
    Sqrt[(Subscript[\[Omega], 0] - \[Omega])^2 + Subscript[\[
        Omega],
    1]^2)];

Print["Iz matrix for spin ", n, " is "];
Print[Iz // MatrixForm];
Print["The energy level matrix for ", n, " Spin is "];  
For[i = 1, i < 2*n + 2, i++, Ix[[i + 1, i]] = Sqrt[(2*n - i + 1)*
    i)/2];
For [i = 1, i < 2*n + 2, i++,
    Ix[[i, i + 1]] = I*Sqrt[(2*n - i + 1)*i]/2];
For [i = 1, i < 2*n + 2, i++, Ix[[i, i]] = 0];
Print["Ix matrix for spin ", n, " is "];
Print[Ix // MatrixForm];
For [i = 1, i < 2*n + 2, i++,
    Iy[[i + 1, i]] = I*Sqrt[(2*n - i + 1)*i]/2]
For [i = 1, i < 2*n + 2, i++,
    Iy[[i, i + 1]] = -I*Sqrt[(2*n - i + 1)*i]/2];
For \[i = 1, i < 2n + 2, i++, Iy[[i, i]] = 0\];

Print["Iy matrix for spin ", n, " is "];
Print[Iy // MatrixForm];

\[\beta\] =
2*ArcSin[(Subscript[\[Omega], 1]/
Sqrt[(Subscript[\[Omega], 0] - \[Omega])^2 +
Subscript[\[Omega], 1]^2])*]

Sin[Sqrt[(Subscript[\[Omega], 0] - \[Omega])^2 +
Subscript[\[Omega], 1]^2]*t/2]];

IzT = MatrixExp[-I*Iz*\[Omega]*t];

Print["The transformation matrix for the states is "];
MT1 = Simplify[IzT . MatrixExp[-I*Iy*\[Beta]*b ]];
Print[MT1 // MatrixForm];

t = \[Tau]*2*Pi/

Sqrt[(Subscript[\[Omega], 0] - \[Omega])^2 + Subscript[\[Omega], 1]^2];

MT1 = Simplify[IzT . MatrixExp[-I*Iy*\[Beta]*b ]];
Print[MT1 // MatrixForm];

Both codes provided above offer the transformation matrices necessary for generating graphical comparisons of spin state probabilities between our research solution and Gottfried’s solution, as detailed in Chapter 4, Section 4.3.
APPENDIX D: CALCULATION AND GRAPHICAL REPRESENTATION OF MULTIPOLE MOMENT ENERGY LEVELS
The following code encompasses calculations for magnetic dipole, electric quadrupole, magnetic octupole, and higher multipole moment energy levels. Furthermore, it can provide computational results for the energy level calculations of $^{14}_7\text{N}$ and $^7\text{Li}$, complementing the hand calculations outlined in the Chapter 4.

```
Print["Let's make sure all variables are cleared at the first"]; ClearAll[n, i, x, y];
OrderNumber = 3;(*This is for multipole q. For example, dipole is 1 here. *)
n = 3/2; (*This is for nuclear spin number I*)
m = 1/2; (*This is for electron spin number J*)
(*The rest of the program will automatically calculate the rest
  when it \n runs.*)
Print["All Clear"];
i = 1;
ID1 = IdentityMatrix[2*n + 1];
Iz = ID1;
Ix = ID1;
Iy = ID1;
IE = ID1;
For[i = 1, i < 2*n + 2, i++,
  IE[[i, i]] = (n - i + 1)*Subscript[\[CapitalOmega], I]];```
Print[ID1 // MatrixForm];
For [i = 1, i < 2*n + 2, i++, Iz[[i, i]] = (n - i + 1)];
Print["Iz matrix for spin ", n, " is "];
Print[Iz // MatrixForm];
Print["The energy level matrix for ", n, " Spin is "];
For[i = 1, i < 2*n + 2, i++, Ix[[i + 1, i]] = Sqrt[(2*n - i + 1)*i]/2];
For [i = 1, i < 2*n + 2, i++,
      Ix[[i, i + 1]] = Sqrt[(2*n - i + 1)*i]/2];
For [i = 1, i < 2*n + 2, i++,
      Ix[[i, i]] = 0];
Print["Ix matrix for spin ", n, " is "]
Print[Ix // MatrixForm];
For [i = 1, i < 2*n + 2, i++,
      Iy[[i + 1, i]] = I*Sqrt[(2*n - i + 1)*i]/2]
For [i = 1, i < 2*n + 2, i++,
      Iy[[i, i + 1]] = -I*Sqrt[(2*n - i + 1)*i]/2];
For [i = 1, i < 2*n + 2, i++,
      Iy[[i, i]] = 0];
Print["Iy matrix for spin ", n, " is "];
Print[Iy // MatrixForm];
j = 1;
ID2 = IdentityMatrix[2*m + 1];
Jz = ID2;
Jx = ID2;

Jy = ID2;

JE = ID2;

For[i = 1, i < 2*m + 2, i++,
    JE[[i, i]] = (m - i + 1)*Subscript[\[CapitalOmega], J]];

Print[JE // MatrixForm];

Print[ID2 // MatrixForm];

For [j = 1, j < 2*m + 2, j++,
    Jz[[j, j]] = (m - j + 1)];

Print["Jz matrix for spin ", m, " is "];

Print[Jz // MatrixForm];

Print["The energy level matrix for ", m, " Spin is "];

For[j = 1, j < 2*m + 2, j++,
    Jx[[j + 1, j]] = Sqrt[(2*m - j + 1)*j]/2];

For [j = 1, j < 2*m + 2, j++,
    Jx[[j, j + 1]] = Sqrt[(2*m - j + 1)*j]/2];

For [j = 1, j < 2*m + 2, j++,
    Jx[[j, j]] = 0];

Print["Jx matrix for spin ", m, " is "]

Print[Jx // MatrixForm];

For [j = 1, j < 2*m + 2, j++,
    Jy[[j + 1, j]] = I*Sqrt[(2*m - j + 1)*j]/2]

For [j = 1, j < 2*m + 2, j++,
    Jy[[j, j]] = 0];

Print["Jy matrix for spin ", m, " is "]

Print[Jy // MatrixForm];
Print["Jy matrix for spin ", m, " is "];
Print[Jy // MatrixForm];
ID3 = IdentityMatrix[(2*n + 1)*(2*m + 1)];
Print[ID3 // MatrixForm];
ITx = ID3;
JTx = ID3;
ITy = ID3;
JTy = ID3;
ITz = ID3;
JTz = ID3;
Print[Ix[[1, 1]]]

H0 = ID3;
For[l = 1, l < 2*n + 2, l++,
 For[g = 1, g < 2*n + 2, g++,
 For[f = 1, f < 2*m + 2, f++,
 For[k = 1, k < 2*m + 2, k++,
 H0[[k + (l - 1)*(2*m + 1), f + (g - 1)*(2*m + 1)]] = (IE[[l, g]] + JE[[k, f]])]]];
For[j = 1, j < (2*n + 1)*(2*m + 1) + 1, j++,
 For[i = 1, i < j, i++, H0[[i, j]] = 0]];
For[l = 1, l < 2*n + 2, l++,
    For[g = 1, g < 2*n + 2, g++,
        For[f = 1, f < 2*m + 2, f++,
            For[k = 1, k < 2*m + 2, k++,
                ITx[[k + (l - 1)*(2*m + 1), f + (g - 1)*(2*m + 1)]] =
                Ix[[l, g]]*ID2[[k, f]]];
          ];
        ];
      ];
    ];
  ];

Print[TensorProduct[Ix, ID2] // MatrixForm];
Print[ITx // MatrixForm];

For[l = 1, l < 2*n + 2, l++,
    For[g = 1, g < 2*n + 2, g++,
        For[f = 1, f < 2*m + 2, f++,
            For[k = 1, k < 2*m + 2, k++,
                ITy[[k + (l - 1)*(2*m + 1), f + (g - 1)*(2*m + 1)]] =
                Iy[[l, g]]*ID2[[k, f]]];
          ];
        ];
      ];

Print[TensorProduct[Iy, ID2] // MatrixForm];
Print[ITy // MatrixForm];

For[l = 1, l < 2*n + 2, l++,
    For[g = 1, g < 2*n + 2, g++,
        For[f = 1, f < 2*m + 2, f++,
            For[k = 1, k < 2*m + 2, k++,
                ITz[[k + (l - 1)*(2*m + 1), f + (g - 1)*(2*m + 1)]] =
                Iz[[l, g]]*ID2[[k, f]]];
          ];
        ];
      ];

Print[TensorProduct[Iz, ID2] // MatrixForm];
Print[Iz // MatrixForm];
Print[ID2 // MatrixForm];
Print[ITz // MatrixForm];

For[l = 1, l < 2*m + 2, l++,
   For[g = 1, g < 2*m + 2, g++,
      For[f = 1, f < 2*n + 2, f++,
         For[k = 1, k < 2*n + 2, k++,
            JTx[[l + (k - 1)*(2*m + 1), g + (f - 1)*(2*m + 1)]] =
            ID1[[k, f]]*Jx[[l, g]]];
   ];
];
Print[TensorProduct[ID1, Jx] // MatrixForm];
Print[JTx // MatrixForm];

For[l = 1, l < 2*m + 2, l++,
   For[g = 1, g < 2*m + 2, g++,
      For[f = 1, f < 2*n + 2, f++,
         For[k = 1, k < 2*n + 2, k++,
            JTy[[l + (k - 1)*(2*m + 1), g + (f - 1)*(2*m + 1)]] =
            ID1[[k, f]]*Jy[[l, g]]];
   ];
];
Print[TensorProduct[ID1, Jy] // MatrixForm];
Print[JTy // MatrixForm];

For[l = 1, l < 2*m + 2, l++,
   For[g = 1, g < 2*m + 2, g++,}
For[f = 1, f < 2*n + 2, f++,
   For[k = 1, k < 2*n + 2, k++,
      JTz[[l + (k - 1)*(2*m + 1), g + (f - 1)*(2*m + 1)]] =
      ID1[[k, f]]*Jz[[l, g]]];
Print[TensorProduct[ID1, Jz] // MatrixForm];
Print[JTz // MatrixForm];
Mmatrix = ID3;
For[j = 1, j < (2*n + 1)*(2*m + 1) + 1, j++, Mmatrix[[j, j]] = 0];
Print[Mmatrix // MatrixForm];
Print["Now we are going to build the Calculation"]
ImpM = FullSimplify[ID3];
getVectorK[n_] := Table[Subscript["K", i], {i, 0, OrderNumber}]
K = getVectorK[OrderNumber];

For[x = 0, x < OrderNumber + 1, x++,
   ImpM = FullSimplify[ID3];
   For[y = 0, y < x, y++,
      ImpM = ImpM . (ITx . JTx + ITy . JTy + ITz . JTz)];
   Print[FullSimplify[ImpM*K[[x + 1]]] // MatrixForm];
   Mmatrix = FullSimplify[Mmatrix + ImpM*K[[x + 1]]];
];
Print["The Mmatrix to " , OrderNumber, " order is ",
   Mmatrix // MatrixForm];
Print[H0 // MatrixForm]
The following code is designed for the numerical calculation and graphical representation of multipole energy levels.

```mathematica
HMatrix = FullSimplify[Mmatrix + H0];
Print[HMatrix // MatrixForm];
Print[Eigenvalues[HMatrix]]; 
Print["The determinant of the matrix is: "];
Print[Det[HMatrix]]; 
Print["The trace of the matrix is: "];
Print[FullSimplify[Tr[HMatrix]]];
```

The following code is designed for the numerical calculation and graphical representation of multipole energy levels. 

```mathematica
Print["Let's make sure all variables are cleared at the first"]; ClearAll[t, w, w0, w1, n, i, MT, x, y, P1, P2, P3, P4, P5, P6, M, w]; Subscript["K", 0] =.; Subscript["K", 1] =.; Subscript["K", 2] =.; Subscript["K", 3] =.; Subscript["K", 4] =.; (*This is for multipole Subscript["K", q]. For example, dipole is Subscript["K", 1] here. The code can add higher multipole moments Subscript["K", q] for more complex system. Here Subscript["K", 0] =. means reset the value for Subscript["K", 0] =.""]
```
\[ Subscript[w, n1] =. ; \\
Subscript[w, n0] =. ; \\
Subscript[w, e1] =. ; \\
Subscript[w, e0] =. ; \\
Subscript[\[CapitalOmega], I] =. ; \\
Subscript[\[CapitalOmega], J] =. ; \\
OrderNumber = \\
3;(*This is for multipole q. For example, dipole is 1 here. *) \\
n = 3/2;(*This is for nuclear spin number I*) \\
m = 1/2; (*This is for electron spin number J*) \\
(*The rest of the program will automatically calculate the rest \\
  when it \ \\
runs.*) \\
Print["All Clear"]; \\
i = 1; \\
ID1 = IdentityMatrix[2*n + 1]; \\
Iz = ID1; \\
Ix = ID1; \\
Iy = ID1; \\
IE = ID1; \\
For[i = 1, i < 2*n + 2, i++,}
IE[[i, i]] = (n - i + 1)\[CapitalOmega]_I];

Print[ID1 // MatrixForm];
For [i = 1, i < 2*n + 2, i++, Iz[[i, i]] = (n - i + 1)];
Print["Iz matrix for spin ", n, " is "];
Print[Iz // MatrixForm];
Print["The energy level matrix for ", n, " Spin is "];
For[i = 1, i < 2*n + 2, i++, Ix[[i + 1, i]] = Sqrt[(2*n - i + 1)*i]/2];
For [i = 1, i < 2*n + 2, i++, Ix[[i, i]] = 0];
Print["Ix matrix for spin ", n, " is "]
Print[Ix // MatrixForm];
For [i = 1, i < 2*n + 2, i++,
    Ix[[i, i + 1]] = Sqrt[(2*n - i + 1)*i]/2];
For [i = 1, i < 2*n + 2, i++, Ix[[i, i]] = 0];
Print["Iy matrix for spin ", n, " is "]
Print[Iy // MatrixForm];
For [i = 1, i < 2*n + 2, i++,
    Iy[[i + 1, i]] = I*Sqrt[(2*n - i + 1)*i]/2]
For [i = 1, i < 2*n + 2, i++,
    Iy[[i, i]] = -I*Sqrt[(2*n - i + 1)*i]/2];
For [i = 1, i < 2*n + 2, i++, Iy[[i, i]] = 0];
Print["Iy matrix for spin ", n, " is "];
Print[Iy // MatrixForm];
j = 1;
ID2 = IdentityMatrix[2*m + 1];
Jz = ID2;
Jx = ID2;
Jy = ID2;
JE = ID2;

For[i = 1, i < 2*m + 2, i++,
    JE[[i, i]] = (m - i + 1)*Subscript[\[CapitalOmega], J]];
Print[JE // MatrixForm];

Print[ID2 // MatrixForm];
For [j = 1, j < 2*m + 2, j++, Jz[[j, j]] = (m - j + 1)];
Print["Jz matrix for spin ", m, " is "];
Print[Jz // MatrixForm];
Print["The energy level matrix for ", m, " Spin is "];
For[j = 1, j < 2*m + 2, j++,
    Jx[[j + 1, j]] = Sqrt[(2*m - j + 1)*j]/2];
For [j = 1, j < 2*m + 2, j++,
    Jx[[j, j + 1]] = Sqrt[(2*m - j + 1)*j]/2];
For [j = 1, j < 2*m + 2, j++,
    Jx[[j, j]] = 0];
Print["Jx matrix for spin ", m, " is 
"]
Print[Jx // MatrixForm];
For [j = 1, j < 2*m + 2, j++,
    Jy[[j + 1, j]] = I*Sqrt[(2*m - j + 1)*j]/2];
For [j = 1, j < 2*m + 2, j++,
    Jy[[j, j + 1]] = -I*Sqrt[(2*m - j + 1)*j]/2];
For [j = 1, j < 2*m + 2, j++, Jy[[j, j]] = 0];
Print["Jy matrix for spin ", m, " is "];
Print[Jy // MatrixForm];
ID3 = IdentityMatrix[(2*n + 1)*(2*m + 1)];
Print[ID3 // MatrixForm];
ITx = ID3;
JTx = ID3;
ITy = ID3;
JTy = ID3;
ITz = ID3;
JTz = ID3;
Print[Ix[[1, 1]]]
H0 = ID3;
For[l = 1, l < 2*n + 2, l++,
  For[g = 1, g < 2*n + 2, g++,
    For[f = 1, f < 2*m + 2, f++,
      For[k = 1, k < 2*m + 2, k++,
      H0[[k + (l - 1)*(2*m + 1), f + (g - 1)*(2*m + 1)]] = (IE[[l, g]] + JE[[k, f]]);]]];
For[j = 1, j < (2*n + 1)*(2*m + 1) + 1, j++,
  For[i = 1, i < j, i++, H0[[i, j]] = 0]];
Print[H0 // MatrixForm];

For[l = 1, l < 2*n + 2, l++,
    For[g = 1, g < 2*n + 2, g++,
        For[f = 1, f < 2*m + 2, f++,
            For[k = 1, k < 2*m + 2, k++,
                ITx[[k + (l - 1)*(2*m + 1), f + (g - 1)*(2*m + 1)]] =
                Ix[[l, g]]*ID2[[k, f]]]]];
    Print[TensorProduct[Ix, ID2] // MatrixForm];
    Print[ITx // MatrixForm];
]

For[l = 1, l < 2*n + 2, l++,
    For[g = 1, g < 2*n + 2, g++,
        For[f = 1, f < 2*m + 2, f++,
            For[k = 1, k < 2*m + 2, k++,
                ITy[[k + (l - 1)*(2*m + 1), f + (g - 1)*(2*m + 1)]] =
                Iy[[l, g]]*ID2[[k, f]]]]];
    Print[TensorProduct[Iy, ID2] // MatrixForm];
    Print[ITy // MatrixForm];
]

For[l = 1, l < 2*n + 2, l++,
    For[g = 1, g < 2*n + 2, g++,
        For[f = 1, f < 2*m + 2, f++,
            For[k = 1, k < 2*m + 2, k++,
                ITz[[k + (l - 1)*(2*m + 1), f + (g - 1)*(2*m + 1)]] =
                Ix[[l, g]]*ID2[[k, f]]]]];
```
Iz[[l, g]]*ID2[[k, f]]];
Print[TensorProduct[Iz, ID2] // MatrixForm];
Print[Iz // MatrixForm];
Print[ID2 // MatrixForm];
Print[ITz // MatrixForm];

For[l = 1, l < 2*m + 2, l++,
  For[g = 1, g < 2*m + 2, g++,
    For[f = 1, f < 2*n + 2, f++,
      For[k = 1, k < 2*n + 2, k++,
        JTx[[l + (k - 1)*(2*m + 1), g + (f - 1)*(2*m + 1)]] =
        ID1[[k, f]]*Jx[[l, g]]];
      Print[TensorProduct[ID1, Jx] // MatrixForm];
      Print[JTx // MatrixForm];
    ]
  ]

For[l = 1, l < 2*m + 2, l++,
  For[g = 1, g < 2*m + 2, g++,
    For[f = 1, f < 2*n + 2, f++,
      For[k = 1, k < 2*n + 2, k++,
        JTy[[l + (k - 1)*(2*m + 1), g + (f - 1)*(2*m + 1)]] =
        ID1[[k, f]]*Jy[[l, g]]];
      Print[TensorProduct[ID1, Jy] // MatrixForm];
      Print[JTy // MatrixForm];
    ]
  ]
```

"
For [g = 1, g < 2*m + 2, g++,
    For [f = 1, f < 2*n + 2, f++,
        For [k = 1, k < 2*n + 2, k++,
            JTz[[l + (k - 1)*(2*m + 1), g + (f - 1)*(2*m + 1)]] =
            ID1[[k, f]]*Jz[[l, g]]]]]];
Print[TensorProduct[ID1, Jz] // MatrixForm];
Print[JTz // MatrixForm];
Mmatrix = ID3;
For [j = 1, j < (2*n + 1)*(2*m + 1) + 1, j++, Mmatrix[[j, j]] =
    0];
Print[Mmatrix // MatrixForm];
Print["Now we are going to build the Calculation"]
ImpM = FullSimplify[ID3];
getVectorK[n_] := Table[Subscript["K", i], {i, 0, OrderNumber}]
K = getVectorK[OrderNumber];

For [x = 0, x < OrderNumber + 1, x++,
    ImpM = FullSimplify[ID3];
    For[y = 0, y < x, y++,
        ImpM = ImpM . (ITx . JTx + ITy . JTy + ITz . JTz)];
    Print[FullSimplify[ImpM*K[[x + 1]] // MatrixForm]];
    Mmatrix = FullSimplify[Mmatrix + ImpM*K[[x + 1]]];
    ];
Print["The Mmatrix to " , OrderNumber, " order is ",
    Mmatrix // MatrixForm];
Print[H0 // MatrixForm]

HMatrix = FullSimplify[Mmatrix + H0];
Print[HMatrix // MatrixForm];
Print[Eigenvalues[HMatrix]];
SOLUTION = Eigenvalues[HMatrix];

(*conditions need to modify for calculation*)

Subscript[\[CapitalOmega], I] = 
Sqrt[(w - Subscript[w, n0])^2 + Subscript[w, n1]^2];
Subscript[\[CapitalOmega], J] = 
Sqrt[(w - Subscript[w, e0])^2 + Subscript[w, e1]^2];
Subscript["K", 0] = 1;
Subscript["K", 1] = 1;
Subscript["K", 2] = 2;
Subscript["K", 3] = 4;

(*This is for multipole Subscript["K", q]. For example, dipole is
 
Subscript["K", 1] here. The code can add higher multipole moments
 
Subscript["K", q] for more complex system.*)

Subscript[w, n1] = 1;
Subscript[w, n0] = 100;
Subscript[w, e1] = 1000;
Subscript[w, e0] = 100000;

(*conditions need to modify for calculation*)

AP = {};

155
KK = {SOLUTION};

(*ReImPlot[SOLUTION, {w, -100, 300}, AxesLabel -> {Style["w", FontColor\\[Rule\] Black, FontSize -> 20], Style["E", FontColor\[Rule] Black, FontSize -> 20]}, PlotStyle\[Rule] Automatic, PlotRange -> Full, TicksStyle\[Rule] Automatic]*)

Do[AppendTo[AP,
  SetPrecision[Part[SOLUTION, i], (* Here,
    we can set up the precision for the graph,
    the initial setting is at 30-digit precision,
    the maximum precision is the MachinePrecision which means the
    exact number*)30(*The precision number*)], {i, 1, (2*n + 1)*(2*m + 1)}];

PP = Plot[AP, {w, 0, 200000},
  AxesLabel -> {Style["\[Omega]", FontColor -> Black,
    FontSize -> 20],
    Style["E", FontColor -> Black, FontSize -> 20]},
  PlotStyle -> Automatic, PlotLegends -> KK, PlotRange -> Full,
  TicksStyle -> {{FontSize -> 20, Black}, {FontSize -> 20, Black}}];

Print[PP]
\( I_x, I_y, \) and \( I_z \) can be represented as delta functions in tensor form.

\[
I_{xcd} = \frac{1}{2} (I_{+cd} + I_{-cd}) = \frac{1}{2} \left( \sqrt{(2I - c + 1)} \delta_{c+1,d} + \sqrt{(2I - c + 2)} (c - 1) \delta_{c-1,d} \right)
\]
\[
I_{ycd} = \frac{1}{2i} (I_{+cd} - I_{-cd}) = \frac{1}{2} \left( -i \sqrt{(2I - c + 1)} \delta_{c+1,d} + i \sqrt{(2I - c + 2)} (c - 1) \delta_{c-1,d} \right)
\]
\[
I_{zcd} = (I + 1 - c) \delta_{c,d}
\]

(E.1)

In here, \( c \) represents the column of the spin matrices, \( d \) represents the row of the spin matrices, and \( I \) represents the nuclear spin value. Therefore, \( H_{\text{eff}} \) can be written as

\[
H_{\text{eff}} = (\omega_0 - \omega) I_z + \omega_1 I_x
\]
\[
= (\omega_0 - \omega) (I + 1 - c) \delta_{c,d}
\]
\[
+ \omega_1 \frac{1}{2} \left( \sqrt{(2I - c + 1)} \delta_{c+1,d} + \sqrt{(2I - c + 2)} (c - 1) \delta_{c-1,d} \right)
\]

(E.2)

The \( H_{\text{diag}} \) can be written as

\[
H_{\text{diag}} = \Omega I_z = \sqrt{(\omega_0 - \omega)^2 + \omega_1^2 - (I + 1 - c) \delta_{c,d}}
\]

(E.3)

By defining \( \omega_0 - \omega = a \) and \( \omega_1^2 = b \), then, \( H_{\text{eff}} \) and \( H_{\text{diag}} \) can be rewritten as

\[
H_{\text{eff}} = a (I + 1 - c) \delta_{c,d} + b \left( \sqrt{(2I - c + 1)} \delta_{c+1,d} + \sqrt{(2I - c + 2)} (c - 1) \delta_{c-1,d} \right)
\]
\[
H_{\text{diag}} = \sqrt{a^2 + 4b^2} (I + 1 - c) \delta_{c,d}
\]

(E.4)

The \( H_{\text{diag}} \) can be written as

\[
H_{\text{diag}} = \begin{pmatrix}
    (I - 1) \sqrt{a^2 + 4b^2} & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
    0 & (I - 1) \sqrt{a^2 + 4b^2} & 0 & 0 & \cdots & 0 & 0 & 0 \\
    \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\
    \vdots & \vdots & \vdots & \ddots & 0 & \cdots & \cdots & \cdots \\
    \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
    \vdots & \vdots & \vdots & \cdots & \ddots & 0 & \cdots & \cdots \\
    0 & 0 & 0 & \cdots & 0 & (I - 1) \sqrt{a^2 + 4b^2} & 0 & 0 \\
    0 & 0 & 0 & \cdots & 0 & 0 & (1 - I) \sqrt{a^2 + 4b^2} & 0 \\
    0 & 0 & 0 & \cdots & 0 & 0 & 0 & -I \sqrt{a^2 + 4b^2}
\end{pmatrix}
\]

(E.5)
The determinant of $H_{\text{diag}}$ can be written as

$$\left(\sqrt{a^2 + 4b^2}\right)^{\frac{2I+1}{2}} \prod_{f=-I}^{I} f$$  \hspace{1cm} (E.6)

The $H_{\text{eff}}$ can be written as:

$$H_{\text{eff}} = 
\begin{pmatrix}
Ia & \sqrt{2I}b & 0 & 0 & \cdots & 0 & 0 & 0 \\
\sqrt{2I}b & (I-1)a & \sqrt{2(2I-1)}b & 0 & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\
0 & 0 & 0 & \cdots & 0 & \sqrt{2(2I-1)}b & (1-I)a & \sqrt{2I}b \\
0 & 0 & 0 & \cdots & 0 & 0 & \sqrt{2I}b & -Ia
\end{pmatrix}$$  \hspace{1cm} (E.7)

In this context, matrices conforming to the structure presented in matrix E.7 will possess eigenvalues identical to those found in matrix E.5. This is attributable to the principle that fixed-angle rotations do not alter the eigenvalues of a matrix.

The procedure of calculating the determinant can be shown as

![Figure E.1: The Situation to Considering the Diagonal Terms for $H_{\text{eff}}$](image)

In figure E.1, all blue blocks represents the $(I + 1 - i) a$ terms any given $i$-th row and $i$-th column.

The function for the terms can be written as
$a^{2I+1} \prod_{i=-I}^{I} (I + 1 - i)$ \hspace{2cm} (E.8)

Figure E.2: The Situation to Considering the Diagonal Terms with 1 Rank 2 Orange Square for $H_{eff}$

In figure E.2, all blue blocks represents the $(I + 1 - i) \ a$ terms any given i-th row and i-th column, one rank 2 orange square represents the off diagonal $b$ terms. The function for the terms can be written as

$$a^{2I-1}b^{2} \sum_{c_{1}=1}^{2I} \left[ \frac{(2I + 1 - c_{1}) c_{1}}{(I + 1 - c_{1})(I - c_{1})} \prod_{i=-I}^{I} (I + 1 - i) \right]$$ \hspace{2cm} (E.9)
In figure E.3, all blue blocks represents the \((I + 1 - i) a\) terms any given \(i\)-th row and \(i\)-th column, two rank 2 orange squares represent the off diagonal \(b\) terms. The function for the terms can be written as

\[
a^{2I-3}b^4 \sum_{c_1=1}^{2I-2} \sum_{c_2=c_1+2}^{2I-2} \left[ \prod_{j=1}^{2} \frac{(2I + 1 - c_j)c_j}{(I + 1 - c_j)(I - c_j)} \prod_{i=-I}^{I} (I + 1 - i) \right] \tag{E.10}
\]

Here, the spin number \(I\) can be integer or half integer. Then the size of the \(H_{eff}\) matrix will not always be divisible by 2. Therefore, the function needs the operation \(\sum_{k=0}^{\lfloor \frac{2I+1}{2} \rfloor}\) to ensure that the \(b\) terms are inside the matrix.
Similarly, in figure E.4, all blue blocks represent the \((I + 1 - i)a\) terms any given i-th row and i-th column, three rank 2 orange squares represents the off diagonal \(b\) terms. The function for the terms can be written as

\[
\begin{align*}
a^{2I-5}b^6 \sum_{c_1=1}^{2I-4} \sum_{c_2=c_1+2}^{2I-2} \sum_{c_3=c_2+2}^{2I} & \left[ \prod_{j=1}^{3} \frac{(2I+1-c_j)c_j}{(I+1-c_j)(I-c_j)} \right] \prod_{i=-I}^{I} (I + 1 - i) \end{align*}
\]  
(E.11)

Figure E.5: The Situation to Considering All Rank 2 Orange Squares for \(H_{eff}\)
The last case, in figure E.5, only consider the $b$ terms in the $H_{eff}$ matrix.

For half integer $I$

$$b^{2I+1} \sum_{c_1=1}^{2n} \sum_{c_2=c_1+2}^{3n} \cdots \sum_{c_j=c_{j-1}+2}^{2I} \prod_{j=1}^{I} (2I + 1 - c_j) c_j$$  \hspace{1cm} (E.12)

For integer $I$

$$ab^{2I} \sum_{c_1=1}^{2n} \sum_{c_2=c_1+2}^{3n} \cdots \sum_{c_j=c_{j-1}+2}^{2I} \left[ \prod_{j=1}^{I} \frac{(2I + 1 - c_j) c_j}{(I + 1 - c_j)(I - c_j)} \prod_{i=-I}^{I} (I + 1 - i) \right]$$  \hspace{1cm} (E.13)

Therefore, the determinant of $H_{eff}$ can be written as

$$\sum_{k=0}^{\frac{2I+1}{2}} \sum_{c_1=1}^{2I-2(k-1)2I-2(k-2)} \cdots \sum_{c_k=c_{k-1}+2}^{2I} \left[ \prod_{j=1}^{k} \frac{(2I + 1 - c_j) c_j}{(I + 1 - c_j)(I - c_j)} a^{2I+1-2k}b^{2k} \prod_{L_i=-I}^{I} L_i \right]$$  \hspace{1cm} (E.14)

Now consider that $a$ or $b$ could be an imaginary number for mathematical purposes. Then the general LK recurrence relation can be written as

$$\left( \sqrt{\pm a^2 + 4b^2} \right)^{2I+1} \prod_{f=-I}^{I} f$$

$$= \sum_{k=0}^{\frac{2I+1}{2}} \sum_{c_1=1}^{2I-2(k-1)2I-2(k-2)} \cdots \sum_{c_k=c_{k-1}+2}^{2I} \left[ \prod_{j=1}^{k} \frac{\pm (2I + 1 - c_j) c_j}{(I + 1 - c_j)(I - c_j)} a^{2I+1-2k}b^{2k} \prod_{L_i=-I}^{I} L_i \right]$$  \hspace{1cm} (E.15)

In addition for a simpler case, if all diagonal terms disappeared. For any integer or half-integer $n$, the math equation below is generated during the set up of the recursion relation:

$$\sum_{c_1=1}^{2n-2(k-1)2n-2(k-2)} \cdots \sum_{c_k=c_{k-1}+2}^{2n} \prod_{i=1}^{k} [(2n + 1 - c_i) c_i]$$  \hspace{1cm} (E.16)

$$= \sum_{f_1=-n}^{n} \cdots \sum_{f_{2k}=-n}^{n} \prod_{i=1}^{2k} f_i$$

163
APPENDIX F: THE HIGH SPIN CASES
In figure F.1, plots of $P_{\frac{5}{2}}(\tau)$ (solid black), $P_{\frac{3}{2}}(\tau)$ (dotted black), $P_{\frac{1}{2}}(\tau)$ (dotted red), $P_{-\frac{1}{2}}(\tau)$ (solid blue), $P_{-\frac{3}{2}}(\tau)$ (dotted blue), and $P_{-\frac{5}{2}}(\tau)$ (dashed black) for $I = \frac{5}{2}$ and $0 \leq \tau = t/T_{n,e} \leq 1$.

In (a), (c), and (e), $C_{\frac{5}{2}}(0) e^{-i\pi/4} = C_{\frac{3}{2}}(0) = C_{\frac{1}{2}}(0) = C_{-\frac{1}{2}}(0) = C_{-\frac{3}{2}}(0) = C_{-\frac{5}{2}}(0) = \frac{1}{\sqrt{6}}$. In (b), (d), and (f), $C_{\frac{5}{2}}(0) = 1$ and $C_m(0) = 0$ for $m \neq \frac{5}{2}$. In (a) and (b), $\omega/\omega_0 = 0.95$, In (c) and (d), $\omega/\omega_0 = 0.99$, and in (e) and (f), $\omega/\omega_0 = 1$. 

Figure F.1: Spin $I = 5/2$
In figure F.2, plots of $P_3(\tau)$ (solid black), $P_2(\tau)$ (dotted black), $P_1(\tau)$ (dotted red), $P_0(\tau)$ (solid blue), $P_{-1}(\tau)$ (dotted blue), $P_{-2}(\tau)$ (dashed black), and $P_{-3}(\tau)$ for $I$ or $J = 3$ and $0 \leq \tau = t/T_{n,e} \leq 1$. In (a), (c), and (e), $C_3(0) e^{-i\pi/4} = C_2(0) = C_1(0) = C_0(0) = C_{-1}(0) = C_{-2}(0) = C_{-3}(0) = \frac{1}{\sqrt{7}}$. In (b), (d), and (f), $C_3(0) = 1$ and $C_m(0) = 0$ for $m \neq 3$. In (a) and (b), $\omega/\omega_0 = 0.95$, In (c) and (d), $\omega/\omega_0 = 0.99$, and in (e) and (f), $\omega/\omega_0 = 1$. 

Figure F.2: Spin $I = 3$
In figure F.3, plots of $P_{\frac{5}{2}}(\tau)$ (dashed blue), $P_{\frac{3}{2}}(\tau)$ (solid black), $P_{\frac{1}{2}}(\tau)$ (dotted black), $P_{-\frac{1}{2}}(\tau)$ (dotted red), $P_{-\frac{3}{2}}(\tau)$ (solid blue), $P_{-\frac{5}{2}}(\tau)$ (dotted blue), $P_{-\frac{7}{2}}(\tau)$ (dashed black), and $P_{-\frac{7}{2}}(\tau)$ (solid red) for $I$ or $J = \frac{7}{2}$ and $0 \leq \tau = t/T_{n,e} \leq 1$. In (a), (c), and (e), $C_{\frac{7}{2}}(0) = C_{\frac{5}{2}}(0) = C_{\frac{3}{2}}(0) = C_{\frac{1}{2}}(0) = C_{-\frac{1}{2}}(0) = C_{-\frac{3}{2}}(0) = C_{-\frac{5}{2}}(0) = C_{-\frac{7}{2}}(0) = 1/\sqrt{8}$. In (b), (d), and (f), $C_{\frac{7}{2}}(0) = 1$ and $C_{m}(0) = 0$ for $m \neq \frac{7}{2}$. In (a) and (b), $\omega/\omega_0 = 0.95$, In (c) and (d), $\omega/\omega_0 = 0.99$, 

Figure F.3: Spin $I = \frac{7}{2}$
and in (e) and (f), $\omega/\omega_0 = 1$.

Figure F.4: Spin $I = 4$

In figure F.4, plots of $P_4 (\tau)$ (dashed blue), $P_3 (\tau)$ (solid black), $P_2 (\tau)$ (dotted black), $P_1 (\tau)$ (dotted red), $P_0 (\tau)$ (solid blue), $P_{-1} (\tau)$ (dotted blue), $P_{-2} (\tau)$ (dashed black), $P_{-3} (\tau)$ (solid red), and $P_{-4} (\tau)$ (dash-dotted black) for $I$ or $J = 4$ and $0 \leq \tau = t/T_{n,e} \leq 1$. In (a), (c), and (e), $C_4 (0) e^{-i\pi/4} = C_3 (0) = C_2 (0) = C_1 (0) = C_0 (0) = C_{-1} (0) = C_{-2} (0) = C_{-3} (0) = C_{-4} (0) =$
In (b), (d), and (f), $C_4(0) = 1$ and $C_m(0) = 0$ for $m 
eq 4$. In (a) and (b), $\omega/\omega_0 = 0.95$, in (c) and (d), $\omega/\omega_0 = 0.99$, and in (e) and (f), $\omega/\omega_0 = 1$.

Figure F.5: Spin $I = 9/2$

In figure F.5, plots of $P_{9/2}(\tau)$ (dashed red), $P_{7/2}(\tau)$ (dashed blue), $P_{5/2}(\tau)$ (solid black), $P_{3/2}(\tau)$ (dotted black), $P_{1/2}(\tau)$ (dotted red), $P_{-1/2}(\tau)$ (solid blue), $P_{-3/2}(\tau)$ (dotted blue), $P_{-5/2}(\tau)$ (dashed black), $P_{-7/2}(\tau)$ (solid red), and $P_{-9/2}(\tau)$ (dash-dotted black) for $I$ or $J = 9/2$ and $0 \leq \tau = t/T_{n,e} \leq 1$. In
(a), (c), and (e), $C_{\frac{1}{2}}(0) e^{-i\pi/4} = C_{\frac{3}{2}}(0) = C_{\frac{5}{2}}(0) = C_{\frac{7}{2}}(0) = C_{\frac{9}{2}}(0) = C_{-\frac{1}{2}}(0) = C_{-\frac{3}{2}}(0) = C_{-\frac{5}{2}}(0) = C_{-\frac{7}{2}}(0) = C_{-\frac{9}{2}}(0) = \frac{1}{\sqrt{10}}$. In (b), (d), and (f), $C_{\frac{3}{2}}(0) = 1$ and $C_m(0) = 0$ for $m \neq \frac{9}{2}$.

In (a) and (b), $\omega/\omega_0 = 0.95$, in (c) and (d), $\omega/\omega_0 = 0.99$, and in (e) and (f), $\omega/\omega_0 = 1$. 
APPENDIX G: REMAINING COMPUTATIONAL GRAPHS FOR
PROBABILITIES AVERAGED OVER A PERIOD
Figure G.1: Spin $I = 2$ and $0.99 \leq \frac{\omega}{\omega_{n0}} \leq 1.01$

In figure G.1, $m = 2$: (solid black), $m = 1$: (dotted black), $m = 0$: (dotted red), $m = -1$: (solid blue), and $m = -2$: (dotted blue). The figure also applies for $J = 2$ with $m$ and $\omega_{n0}$ respectively replaced by $\bar{m}$ and $\omega_{e0}$. 

172
In figure G.2, $m = \frac{5}{2}$: (solid black), $m = \frac{3}{2}$: (dotted black), $m = \frac{1}{2}$: (dotted red), $m = -\frac{1}{2}$: (solid blue), $m = -\frac{3}{2}$: (dotted blue), and $m = -\frac{5}{2}$: (dotted black). In part (a), each $C_m(0) = \frac{1}{\sqrt{6}}$. In part (b), $C_{\frac{5}{2}}(0) = e^{i(\frac{\pi}{2} + 0)} / \sqrt{6}$ and the other $C_m(0) = \frac{1}{\sqrt{6}}$. In part (c), the $C_m(0) = e^{i\phi_m} / \sqrt{6}$, where each phase $\phi_m$ is a random number between 0 to $2\pi$. In part (d), $C_{\frac{5}{2}}(0) = 1$ and the other $C_m(0) = 0$. 
Figure G.3: Spin $I = \frac{7}{2}$ and $0.995 \leq \frac{\omega}{\omega_{n,e}} \leq 1.005$

In figure G.3, $m = 3$: (solid black), $m = 2$: (dotted black), $m = 1$: (dotted red), $m = 0$: (solid blue), $m = -1$: (dotted blue), $m = -2$: (dotted black), and $m = -3$: (solid red). In part (a), each $C_m (0) = \frac{1}{\sqrt{7}}$. In part (b), $C_3 (0) = e^{i(\frac{7}{2} + 0.2)}/\sqrt{7}$ and the other $C_m (0) = \frac{1}{\sqrt{7}}$. In part (c), the $C_m (0) = e^{i\phi_m}/\sqrt{7}$, where each phase $\phi_m$ is a random number between 0 to $2\pi$. In part (d), $C_3 (0) = 1$ and the other $C_m (0) = 0$. 
Figure G.4: Spin \( I = \frac{7}{2} \) and \( 0.995 \leq \frac{\omega}{\omega_{n,c0}} \leq 1.005 \)

In figure G.4, \( m = \frac{7}{2} \): (dashed blue), \( m = \frac{5}{2} \): (solid black), \( m = \frac{3}{2} \): (dotted black), \( m = \frac{1}{2} \): (dotted red), \( m = -\frac{1}{2} \): (solid blue), \( m = -\frac{3}{2} \): (dotted blue), \( m = -\frac{5}{2} \): (dotted black), and \( m = -\frac{7}{2} \): (solid red). In part (a), each \( C_m (0) = \frac{1}{\sqrt{8}} \). In part (b), \( C_{\frac{7}{2}} (0) = e^{i(\frac{\pi}{2} + 0.2)}/\sqrt{8} \) and the other \( C_m (0) = \frac{1}{\sqrt{8}} \).

In part (c), the \( C_m (0) = e^{i\phi_m}/\sqrt{8} \), where each phase \( \phi_m \) is a random number between 0 to 2\( \pi \). In part (d), \( C_{\frac{7}{2}} (0) = 1 \) and the other \( C_m (0) = 0 \).
Figure G.5: Spin $I = 4$ and $0.995 \leq \frac{\omega}{\omega_{n,e}} \leq 1.005$

In figure G.5, $m = 4$: (dashed blue), $m = 3$: (solid black), $m = 2$: (dotted black), $m = 1$: (dotted red), $m = 0$: (solid blue), $m = -1$: (dotted blue), $m = -2$: (dotted black), $m = -3$: (solid red), and $m = -4$: (dashed-dotted black). In part (a), each $C_m(0) = \frac{1}{3}$. In part (b), $C_4(0) = e^{i(\frac{\pi}{2} + 0.2)}/3$ and the other $C_m(0) = \frac{1}{3}$. In part (c), the $C_m(0) = e^{i\phi_m}/3$, where each phase $\phi_m$ is a random number between 0 to 2$\pi$. In part (d), $C_4(0) = 1$ and the other $C_m(0) = 0$. 

176
In figure G.6, $m = \frac{9}{2}$: (dashed red), $m = \frac{7}{2}$: (dashed blue), $m = \frac{5}{2}$: (solid black), $m = \frac{3}{2}$: (dotted black), $m = \frac{1}{2}$: (dotted red), $m = -\frac{1}{2}$: (solid blue), $m = -\frac{3}{2}$: (dotted blue), $m = -\frac{5}{2}$: (dotted black), $m = -\frac{7}{2}$: (solid red), and $m = -\frac{9}{2}$: (dashed-dotted black). In part (a), each $C_m(0) = \frac{1}{\sqrt{10}}$. In part (b), $C_{\frac{9}{2}}(0) = e^{i\left(\frac{\pi}{2} + 0.2\right)}/\sqrt{10}$ and the other $C_m(0) = \frac{1}{\sqrt{10}}$. In part (c), the $C_m(0) = e^{i\phi_m}/\sqrt{10}$, where each phase $\phi_m$ is a random number between 0 to $2\pi$. In part (d), $C_{\frac{9}{2}}(0) = 1$ and the other $C_m(0) = 0$. 

Figure G.6: Spin $I = \frac{9}{2}$ and $0.995 \leq \frac{\omega}{\omega_{n,e}} \leq 1.005$
APPENDIX H: TIME-DEPENDENT PERTURBATIONS
The transformed time-dependent perturbations are listed below:

The nuclear cases,

\[ \delta \hat{V}_{n1}(t) = -\omega_{n1} \sin(\omega t) \left[ J_y \cos(\omega t) + \sin(\omega t) (J_x \cos(\beta_n) + J_z \sin(\beta_n)) \right] \]

\[ + \omega_{n1} \left[ \cos(\omega t) (J_x \cos(\beta_n) + J_z \sin(\beta_n)) - J_y \sin(\omega t) \right] \sum_{p=2}^{\infty} a_p \cos[p\omega (t - t_0)] \]

(\text{H.1})

\[ \delta \hat{V}_{n2}(t) = 2\omega_{n1} \sin(\omega t) \left[ J_z \cos(\theta) \left( J_x \cos(\beta_n) - \sin(\theta) \sin(\beta_n) \cos(\omega t) \right) \right. \]

\[ - \left. J_x \left( \cos(\theta) \sin(\beta_n) + \sin(\theta) \cos(\beta_n) \cos(\omega t) \right) - J_y \sin(\theta) \sin(\omega t) \right] \}

The electronic cases,

\[ \delta \hat{V}_{e1}(t) = -\omega_{e1} \sin(\omega t) \left[ J_y \cos(\omega t) + \sin(\omega t) (J_x \cos(\beta_e) + J_z \sin(\beta_e)) \right] \]

\[ + \omega_{e1} \left[ \cos(\omega t) (J_x \cos(\beta_e) + J_z \sin(\beta_e)) - J_y \sin(\omega t) \right] \sum_{p=2}^{\infty} a_p \cos[p\omega (t - t_0)] \]

(\text{H.2})

\[ \delta \hat{V}_{e2}(t) = 2\omega_{e1} \sin(\theta) \cos(\omega t) \left[ J_z \cos(\theta) \cos(\beta_e) - \sin(\theta) \sin(\beta_e) \cos(\omega t) \right] \]

\[ - \left. J_x \left( \cos(\theta) \sin(\beta_n) + \sin(\theta) \cos(\beta_n) \cos(\omega t) \right) - J_y \sin(\theta) \sin(\omega t) \right] \} \]
APPENDIX I: MATRIX REDUCTIONS
Due to the size of the matrix, assume

\[
A_1 = \mu_1 + \Omega^{1, \frac{3}{2}}_{1, \frac{1}{2}} - \lambda, \quad A_2 = \mu_2 + \Omega^{1, \frac{3}{2}}_{1, \frac{3}{2}} - \lambda, \quad A_3 = \mu_3 + \Omega^{1, \frac{3}{2}}_{1, -\frac{1}{2}} - \lambda, \quad A_4 = \mu_4 + \Omega^{1, \frac{3}{2}}_{1, -\frac{3}{2}} - \lambda \\
A_5 = \mu_5 + \Omega^{0, \frac{3}{2}}_{0, \frac{1}{2}} - \lambda, \quad A_6 = \mu_6 + \Omega^{0, \frac{3}{2}}_{0, \frac{3}{2}} - \lambda, \quad A_7 = \mu_6 + \Omega^{0, \frac{3}{2}}_{0, -\frac{1}{2}} - \lambda, \quad A_8 = \mu_5 + \Omega^{0, \frac{3}{2}}_{0, -\frac{3}{2}} - \lambda \\
A_9 = \mu_4 + \Omega^{1, \frac{3}{2}}_{-1, \frac{1}{2}} - \lambda, \quad A_{10} = \mu_3 + \Omega^{1, \frac{3}{2}}_{-1, \frac{3}{2}} - \lambda, \\
A_{11} = \mu_2 + \Omega^{1, \frac{3}{2}}_{-1, -\frac{1}{2}} - \lambda, \quad A_{12} = \mu_1 + \Omega^{1, \frac{3}{2}}_{-1, -\frac{3}{2}} - \lambda
\]

for the matrix reduction process.

Figure I.1: I=1 and J=3/2 Original Magnetic Dipole and Electric Quadrupole Moment Matrix

Here, the original matrix has been color coded for demonstration purposes. The orange-colored blocks represent any \(A_i\) terms on the diagonal. And the green colored blocks represent any of the
$\Gamma_i$ terms. The blue-colored blocks represent the $\delta$ terms. Finally, empty blocks represent zeros. Then the matrix can be reduced to

![Matrix Diagram](image)

Figure I.2: The Matrices After First Reduction from the Rank-12 Matrix

Therefore, the original matrix can be separated into two matrices, one $2 \times 2$ matrix and one $10 \times 10$ matrix.

The $2 \times 2$ matrix can be easily solved for the $\lambda$ values.

$$\lambda_{1,12} = K_0 + \frac{3}{2} K_1 + \frac{9}{4} K_2 \pm \Omega_I \pm \frac{3}{2} \Omega_J$$  \hspace{1cm} (I.2)

The remaining $10 \times 10$ matrix can be written as
Here, row-4 of the matrix is moved to row-2, then row-2 and row-3 moved one row after correspondingly. Therefore, $A_3$, $A_4$, $\Gamma_2$, $\Gamma_3$, and $\delta$ to change to $-A_3$, $-A_4$, $-\Gamma_2$, $-\Gamma_3$, and $-\delta$; but $\Gamma_1$ and $A_5$ remain unchanged for the elements that moved during this process. The rules are, if the initial row or column move an even number of rows or columns, the sign of each elements inside the initial row or column do not change. However, if the initial row or column moved an odd number of rows or columns, then the elements inside the initial row or column have to change their signs.

Now, column-4 can move to column-2, then column-2 and column-3 can move 1 column to the right correspondingly.
After the second transformation, the column-2 and column-3 elements are moved to column-3 and column-4. $\Gamma_1$ and $A_5$ remain unchanged. $-A_3$ and $-A_4$ are changed back to $A_3$ and $A_4$. $\Gamma_2$, $\Gamma_3$, $\delta$ are changed to $-\Gamma_2$, $-\Gamma_3$, $-\delta$.

The process will now be demonstrated with multiple row changes simultaneously applied for matrix transformation. The original row-5 to the row-4, the original row-8 to the row-5, the original row-4 to row-6, the original row-6 to row-7, the original row-7 to row-8.

Therefore, $-\Gamma_2$, $A_6$, and $\Gamma_3$ in the original row-5; $-\Gamma_3$, $A_6$, and $\Gamma_3$ in the original row-6; $-\delta$, $\Gamma_3$, and $A_9$ in the original row-8; all of them change their signs. However, the rest of the moved rows...
remain with the it signs unchanged. Move the original column-5 to column-4, moved the original column-8 to column-5, move the original column-4 to column-6, move the original column-6 to column-7, and move the original column-7 to column-8.

Finally, move the original column-8 to column-9, and the original column-9 to column-8. Then move the moved row-8 to row-9 and the moved row-9 to row-8.

Therefore, the matrix can be reduced to four small matrices.
\[
\begin{pmatrix}
A_2 & \Gamma_1 \\
\Gamma_1 & A_5
\end{pmatrix} =
\begin{pmatrix}
\mu_2 + \Omega_{1/2}^{1/2} - \lambda & \Gamma_1 \\
\Gamma_1 & \mu_5 + \Omega_{0,2}^{1/2} - \lambda
\end{pmatrix}
\] (I.3)

The determinant can be written as

\[
\begin{split}
&\left( \mu_2 + \Omega_{1/2}^{1/2} - \lambda \right) \left( \mu_5 + \Omega_{0,2}^{1/2} - \lambda \right) - \Gamma_1^2 \\
= &\mu_2 \mu_5 + \mu_2 \Omega_{0,2}^{1/2} - \mu_2 \lambda + \Omega_{1/2}^{1/2} \mu_5 + \Omega_{1/2}^{1/2} \Omega_{0,2}^{1/2} - \Omega_{1/2}^{1/2} \lambda - \lambda \mu_5 - \lambda \Omega_{0,2}^{1/2} + \lambda^2
\end{split}
\] (I.4)

Then, \( \lambda_{2,5} \) could be found

\[
\lambda_{2,5} = \frac{\left( \mu_2 + \mu_5 + \Omega_{1,1/2}^{1/2} + \Omega_{0,1/2}^{1/2} \right)}{2} \\
\pm \sqrt{\left( \mu_2 + \mu_5 + \Omega_{1,1/2}^{1/2} + \Omega_{0,1/2}^{1/2} \right)^2 - 4 \left( \mu_2 \mu_5 + \mu_2 \Omega_{0,2}^{1/2} + \mu_5 \Omega_{1,1/2}^{1/2} \right)}
\] (I.5)

Similarly,

\[
\begin{pmatrix}
A_8 & \Gamma_1 \\
\Gamma_1 & A_{11}
\end{pmatrix} =
\begin{pmatrix}
\mu_5 + \Omega_{0,-1/2}^{1/2} - \lambda & \Gamma_1 \\
\Gamma_1 & \mu_2 + \Omega_{-1,-1/2}^{1/2} - \lambda
\end{pmatrix}
\] (I.6)

The determinant can be written as

\[
\begin{split}
&\left( \mu_5 + \Omega_{0,-1/2}^{1/2} - \lambda \right) \left( \mu_2 + \Omega_{-1,-1/2}^{1/2} - \lambda \right) - \Gamma_1^2 \\
= &\mu_5 \mu_2 + \mu_5 \Omega_{-1,-1/2}^{1/2} - \mu_5 \lambda + \Omega_{0,-1/2}^{1/2} \mu_2 + \Omega_{0,-1/2}^{1/2} \Omega_{-1,-1/2}^{1/2} - \Omega_{0,-1/2}^{1/2} \Omega_{-1,-1/2}^{1/2} - \Omega_{0,-1/2}^{1/2} \lambda - \lambda \mu_2 - \lambda \Omega_{-1,-1/2}^{1/2} + \lambda^2
\end{split}
\] (I.7)

Then, \( \lambda_{8,11} \) could be found

186
\[ \lambda_{8,11} = \frac{\left( \mu_5 + \mu_2 + \Omega^{1/2}_{-1,-1/2} + \Omega^{1/2}_{0,-1/2} \right)}{2} \pm \sqrt{\left( \mu_5 + \mu_2 + \Omega^{1/2}_{-1,-1/2} + \Omega^{1/2}_{0,-1/2} \right)^2 - 4 \left( \mu_5 \mu_2 + \mu_5 \Omega^{1/2}_{-1,-1/2} + \mu_2 \Omega^{1/2}_{0,-1/2} \right)} \]  

(1.8)

Next, a rank 3 matrix

\[
\begin{pmatrix}
A_3 & \Gamma_2 & \delta \\
\Gamma_2 & A_6 & \Gamma_3 \\
\delta & \Gamma_3 & A_9
\end{pmatrix} =
\begin{pmatrix}
\mu_3 + \Omega^{1/2}_{1,-1/4} - \lambda & \Gamma_2 & \delta \\
\Gamma_2 & \mu_6 + \Omega^{1/2}_{0,1/2} - \lambda & \Gamma_3 \\
\delta & \Gamma_3 & \mu_4 + \Omega^{1/2}_{-1,1/2} - \lambda
\end{pmatrix}
\]  

(1.9)

The determinant can be written as
\( \left( \mu_3 + \Omega_{1,\frac{3}{2}} \right) \left( \mu_6 + \Omega_{0,\frac{3}{2}} \right) - \lambda \) 
\[
\begin{vmatrix}
\Delta_3 & \mu_3 + \Omega_{1,\frac{3}{2}} \Delta_3 & - \lambda \\
\Delta_3 & \mu_4 + \Omega_{1,\frac{3}{2}} & - \lambda \\
- \lambda & \mu_6 + \Omega_{0,\frac{3}{2}} & - \lambda & \Delta_3
\end{vmatrix}
\]

\[
= \left( \mu_3 + \Omega_{1,\frac{3}{2}} \right) \left[ \left( \mu_6 + \Omega_{0,\frac{3}{2}} \right) - \lambda \left( \mu_4 + \Omega_{1,\frac{3}{2}} - \lambda \right) - \Gamma_3 \right] - \Gamma_3 \left( \mu_4 + \Omega_{1,\frac{3}{2}} - \lambda \right) + \Gamma_2 \delta + \delta \Gamma_3 - \left( \mu_6 + \Omega_{0,\frac{3}{2}} - \lambda \right) \delta^2
\]

\[
= \left( \mu_3 + \Omega_{1,\frac{3}{2}} \right) \left[ \mu_6 \mu_4 + \mu_6 \Omega_{1,\frac{3}{2}} - \mu_6 \lambda + \mu_4 \Omega_{0,\frac{3}{2}} + \Omega_{1,\frac{3}{2}} \Omega_{1,\frac{3}{2}} - \Omega_{1,\frac{3}{2}} \lambda \\
- \mu_4 \lambda - \Omega_{1,\frac{3}{2}} \lambda + \lambda^2 - \Gamma_3 \right] - \Gamma_2 \mu_4 - \Gamma_2 \Omega_{1,\frac{3}{2}} + \Gamma_2 \lambda + \Gamma_2 \delta + \delta \Gamma_2 \Gamma_3
\]

\[
- \delta^2 \mu_6 - \delta^2 \Omega_{0,\frac{3}{2}} + \delta^2 \lambda
\]

(I.10)

Sort out terms by powers of \( \lambda \). The \( \lambda^0 \) terms can be written as

\[
Z_1 = \mu_3 \mu_4 \mu_6 + \mu_3 \mu_6 \Omega_{1,\frac{3}{2}} + \mu_4 \Omega_{0,\frac{3}{2}} + \mu_3 \Omega_{0,\frac{3}{2}} \Omega_{1,\frac{3}{2}} - \mu_3 \Gamma_3 + \mu_4 \mu_4 \Omega_{1,\frac{3}{2}} + \mu_6 \Omega_{-1,\frac{3}{2}} \Omega_{1,\frac{3}{2}}
\]

\[
+ \mu_4 \Omega_{0,\frac{3}{2}} \Omega_{1,\frac{3}{2}} + \Omega_{1,\frac{3}{2}} \Omega_{1,\frac{3}{2}} - \Gamma_3 \Omega_{1,\frac{3}{2}} - \Gamma_2 \mu_4 - \Gamma_2 \Omega_{1,\frac{3}{2}} + 2 \Gamma_2 \Gamma_3 \delta
\]

\[
- \delta^2 \mu_6 - \delta^2 \Omega_{0,\frac{3}{2}}
\]

(I.11)

The \( \lambda^1 \) terms can be written as
\[
\lambda Y_1 = \lambda \left( -\mu_3 \mu_6 - \mu_3 \Omega_{0,\frac{1}{2}}^{1, \frac{3}{2}} - \mu_3 \mu_4 - \mu_3 \Omega_{-1,\frac{1}{2}}^{1, \frac{3}{2}} - \mu_6 \Omega_{1,\frac{1}{2}}^{1, \frac{3}{2}} - \Omega_{0,\frac{1}{2}}^{1, \frac{3}{2}} \Omega_{-1,\frac{1}{2}}^{1, \frac{3}{2}} - \mu_4 \Omega_{1,\frac{1}{2}}^{1, \frac{3}{2}} - \Omega_{-1,\frac{1}{2}}^{1, \frac{3}{2}} \Omega_{1,\frac{1}{2}}^{1, \frac{3}{2}} \\
- \mu_4 \mu_6 - \mu_6 \Omega_{-1,\frac{1}{2}}^{1, \frac{3}{2}} - \mu_4 \Omega_{0,\frac{1}{2}}^{1, \frac{3}{2}} - \Omega_{0,\frac{1}{2}}^{1, \frac{3}{2}} \Omega_{1,-\frac{1}{2}}^{1, \frac{3}{2}} - \mu_4 \mu_6 - \mu_6 \Omega_{-1,\frac{1}{2}}^{1, \frac{3}{2}} + \mu_4 \Omega_{0,\frac{1}{2}}^{1, \frac{3}{2}} - \Omega_{0,\frac{1}{2}}^{1, \frac{3}{2}} \Omega_{-1,\frac{1}{2}}^{1, \frac{3}{2}} \\
+ \Gamma_3^2 + \Gamma_2^2 + \delta^2 \right)
\]  

(I.12)

The \( \lambda^2 \) terms can be written as

\[
\lambda^2 X_1 = \lambda^2 \left( \mu_3 + \Omega_{1,\frac{1}{2}}^{1, \frac{3}{2}} + \mu_6 + \Omega_{0,\frac{1}{2}}^{1, \frac{3}{2}} + \mu_4 + \Omega_{-1,\frac{1}{2}}^{1, \frac{3}{2}} \right)
\]  

(I.13)

The \( \lambda^3 \) term can be written as \( -\lambda^3 \).

Therefore, the general form can written as \( -\lambda^3 + X \lambda^2 + Y \lambda + Z \), since the rank 10 matrix also has another rank 3 matrix with similar structure. Therefore, it can proceed with the next rank 3 matrix first, and then calculate the \( \lambda \) value.

The last separated matrix can be written as

\[
\begin{pmatrix}
A_4 & \Gamma_3 & \delta \\
\Gamma_3 & A_7 & \Gamma_2 \\
\delta & \Gamma_2 & A_{10}
\end{pmatrix}
= 
\begin{pmatrix}
\mu_4 + \Omega_{1,\frac{1}{2}}^{1, \frac{3}{2}} - \lambda & \Gamma_3 & \delta \\
\Gamma_3 & \mu_6 + \Omega_{0,\frac{1}{2}}^{1, \frac{3}{2}} - \lambda & \Gamma_2 \\
\delta & \Gamma_2 & \mu_3 + \Omega_{-1,\frac{1}{2}}^{1, \frac{3}{2}} - \lambda
\end{pmatrix}
\]  

(I.14)

The determinant can be written as
\[
\begin{vmatrix}
\mu_4 + \Omega_{1,-\frac{3}{2}}^{1,\frac{3}{2}} - \lambda \\
\mu_6 + \Omega_{0,-\frac{3}{2}}^{1,\frac{3}{2}} - \lambda - \Gamma_2 \\
\mu_3 + \Omega_{-1,\frac{1}{2}}^{1,\frac{3}{2}} - \lambda
\end{vmatrix}
\begin{vmatrix}
\Gamma_2 \\
\mu_3 + \Omega_{-1,\frac{1}{2}}^{1,\frac{3}{2}} - \lambda \\
\Gamma_2
\end{vmatrix}
\begin{vmatrix}
\delta \\
\mu_3 + \Omega_{0,-\frac{3}{2}}^{1,\frac{3}{2}} - \lambda
\end{vmatrix}
\begin{vmatrix}
\Gamma_3 \\
\delta \\
\mu_6 + \Omega_{0,-\frac{3}{2}}^{1,\frac{3}{2}} - \lambda
\end{vmatrix}
\]

\[
= \left( \mu_4 + \Omega_{1,-\frac{3}{2}}^{1,\frac{3}{2}} - \lambda \right) \left[ \left( \mu_6 + \Omega_{0,-\frac{3}{2}}^{1,\frac{3}{2}} - \lambda \right) \left( \mu_3 + \Omega_{-1,\frac{1}{2}}^{1,\frac{3}{2}} - \lambda \right) - \Gamma_2^2 \right]
- \Gamma_3 \left[ \Gamma_3 \left( \mu_3 + \Omega_{1,-\frac{3}{2}}^{1,\frac{3}{2}} - \lambda \right) - \Gamma_2 \delta \right] + \delta \left[ \Gamma_3 \Gamma_2 - \left( \mu_6 + \Omega_{0,-\frac{3}{2}}^{1,\frac{3}{2}} - \lambda \right) \delta \right]
\]

\[
\begin{align*}
\lambda^3 - \Gamma_3 \left( \mu_3 + \Gamma_3 \Omega_{1,\frac{1}{2}}^{1,\frac{3}{2}} - \delta - \Gamma_2 \delta \right)
+ \delta \left[ \Gamma_2 \Gamma_3 - \mu_6 \delta - \Omega_{0,-\frac{3}{2}}^{1,\frac{3}{2}} \delta + \delta \lambda \right]
\end{align*}
\]

\[= \mu_3 \mu_4 \mu_6 + \mu_4 \mu_6 \Omega_{-1,\frac{3}{2}}^{1,\frac{3}{2}} - \mu_4 \mu_6 \lambda + \mu_3 \mu_4 \Omega_{0,\frac{3}{2}}^{1,\frac{3}{2}} + \mu_4 \Omega_{-1,\frac{3}{2}}^{1,\frac{3}{2}} \Omega_{0,\frac{3}{2}}^{1,\frac{3}{2}} - \mu_4 \Omega_{0,\frac{3}{2}}^{1,\frac{3}{2}} \lambda - \mu_3 \mu_4 \lambda
\]

\[
- \mu_4 \Omega_{-1,\frac{3}{2}}^{1,\frac{3}{2}} \lambda + \mu_4 \lambda^2 - \mu_4 \Gamma_2 + \mu_3 \mu_6 \Omega_{1,\frac{3}{2}}^{1,\frac{3}{2}} + \mu_6 \Omega_{1,\frac{3}{2}}^{1,\frac{3}{2}} \Omega_{-1,\frac{3}{2}}^{1,\frac{3}{2}} - \mu_6 \Omega_{1,\frac{3}{2}}^{1,\frac{3}{2}} \lambda + \mu_3 \Omega_{0,\frac{3}{2}}^{1,\frac{3}{2}} \Omega_{-1,\frac{3}{2}}^{1,\frac{3}{2}}
\]

\[
+ \Omega_{-1,\frac{3}{2}}^{1,\frac{3}{2}} \Omega_{1,\frac{3}{2}}^{1,\frac{3}{2}} - \Omega_{-1,\frac{3}{2}}^{1,\frac{3}{2}} \Omega_{1,\frac{3}{2}}^{1,\frac{3}{2}} \lambda - \mu_3 \Omega_{-1,\frac{3}{2}}^{1,\frac{3}{2}} \lambda - \Omega_{-1,\frac{3}{2}}^{1,\frac{3}{2}} \Omega_{1,\frac{3}{2}}^{1,\frac{3}{2}} \lambda + \Omega_{1,\frac{3}{2}}^{1,\frac{3}{2}} \lambda^2 - \Gamma_2 \Omega_{1,\frac{3}{2}}^{1,\frac{3}{2}}
\]

\[
- \mu_3 \mu_6 \lambda - \mu_6 \Omega_{-1,\frac{3}{2}}^{1,\frac{3}{2}} \lambda + \mu_6 \lambda^2 - \mu_3 \Omega_{0,\frac{3}{2}}^{1,\frac{3}{2}} \lambda - \Omega_{0,\frac{3}{2}}^{1,\frac{3}{2}} \Omega_{-1,\frac{3}{2}}^{1,\frac{3}{2}} \lambda + \Omega_{0,\frac{3}{2}}^{1,\frac{3}{2}} \lambda^2 + \mu_3 \lambda^2 + \Omega_{0,\frac{3}{2}}^{1,\frac{3}{2}} \lambda^2
\]

\[
- \lambda^3 + \Gamma_2 \lambda \Gamma_3 - \Gamma_3 \Omega_{1,\frac{3}{2}}^{1,\frac{3}{2}} + \Gamma_2 \lambda + 2 \Gamma_2 \Gamma_3 \delta - \mu_6 \delta^2 - \Omega_{0,\frac{3}{2}}^{1,\frac{3}{2}} \delta^2 + \delta^2 \lambda
\]

Sort out terms by \( \lambda \). The \( \lambda^0 \) terms can be written as

\[
Z_2 = \mu_3 \mu_4 \mu_6 + \mu_4 \mu_6 \Omega_{-1,\frac{3}{2}}^{1,\frac{3}{2}} + \mu_3 \mu_4 \Omega_{0,\frac{3}{2}}^{1,\frac{3}{2}} + \mu_4 \Omega_{-1,\frac{3}{2}}^{1,\frac{3}{2}} \Omega_{0,\frac{3}{2}}^{1,\frac{3}{2}} - \mu_4 \Gamma_2^2 + \mu_3 \mu_6 \Omega_{1,\frac{3}{2}}^{1,\frac{3}{2}} + \mu_6 \Omega_{1,\frac{3}{2}}^{1,\frac{3}{2}} \Omega_{0,\frac{3}{2}}^{1,\frac{3}{2}} + \mu_3 \Omega_{0,\frac{3}{2}}^{1,\frac{3}{2}} \Omega_{1,\frac{3}{2}}^{1,\frac{3}{2}} + \mu_6 \Omega_{-1,\frac{3}{2}}^{1,\frac{3}{2}} \Omega_{0,\frac{3}{2}}^{1,\frac{3}{2}} - \Gamma_2 \Omega_{1,\frac{3}{2}}^{1,\frac{3}{2}} + \Gamma_3 \mu_3 - \Gamma_3 \Omega_{1,\frac{3}{2}}^{1,\frac{3}{2}}
\]

\[+ 2 \Gamma_2 \Gamma_3 \delta - \mu_6 \delta^2 - \Omega_{0,\frac{3}{2}}^{1,\frac{3}{2}} \delta^2
\]

The \( \lambda^1 \) terms can be written as
One may list the indices for $\lambda$ in equation I.9 and I.14 can be written as follows:

For example, $\lambda_6$ contains $X_1$. Therefore, similar to the case of equation I.9, the equation for $\lambda$ resulting from equation I.14 can be written as $-\lambda^3 + X_2\lambda^2 + Y_2\lambda + Z_2 = 0$.

Based on the general cubic formula for $ax^3 + bx^2 + cx + d = 0$, the general cubic solutions can be written as,

\[
\begin{align*}
\lambda_1 &= \frac{-b}{3a} - \frac{1}{3a} \sqrt[3]{\frac{1}{2} \left[ 2b^3 - 9abc + 27a^2d + \sqrt{\left(2b^3 - 9abd + 27a^2d\right) - 4(b^2 - 3ac)^3} \right]} \\
&\quad - \frac{1}{3a} \sqrt[3]{\frac{1}{2} \left[ 2b^3 - 9abc + 27a^2d - \sqrt{\left(2b^3 - 9abd + 27a^2d\right) - 4(b^2 - 3ac)^3} \right]} \\
\lambda_2 &= \frac{-b}{3a} + \frac{1 + i\sqrt{3}}{6a} \sqrt[3]{\frac{1}{2} \left[ 2b^3 - 9abc + 27a^2d + \sqrt{\left(2b^3 - 9abd + 27a^2d\right) - 4(b^2 - 3ac)^3} \right]} \\
&\quad - \frac{1 - i\sqrt{3}}{6a} \sqrt[3]{\frac{1}{2} \left[ 2b^3 - 9abc + 27a^2d - \sqrt{\left(2b^3 - 9abd + 27a^2d\right) - 4(b^2 - 3ac)^3} \right]} \\
\lambda_3 &= \frac{-b}{3a} + \frac{1 - i\sqrt{3}}{6a} \sqrt[3]{\frac{1}{2} \left[ 2b^3 - 9abc + 27a^2d + \sqrt{\left(2b^3 - 9abd + 27a^2d\right) - 4(b^2 - 3ac)^3} \right]} \\
&\quad - \frac{1 + i\sqrt{3}}{6a} \sqrt[3]{\frac{1}{2} \left[ 2b^3 - 9abc + 27a^2d - \sqrt{\left(2b^3 - 9abd + 27a^2d\right) - 4(b^2 - 3ac)^3} \right]}
\end{align*}
\] (I.19)
$Y_1$, and $Z_1$.

$$\lambda_m = \frac{\sqrt[3]{2X_n^3 + 3\sqrt{3}X_n^3Z_n - X_n^2Y_n^2 + 18X_nY_nZ_n - 4Y_n^3 + 27Z_n^2 + 9X_nY_n + 27Z_n}}{3\sqrt[3]{2}}$$

$$- \frac{\sqrt[3]{2X_n^3 + 3\sqrt{3}X_n^3Z_n - X_n^2Y_n^2 + 18X_nY_nZ_n - 4Y_n^3 + 27Z_n^2 + 9X_nY_n + 27Z_n}}{3\sqrt[3]{2(-X_n^2 - 3Y_n)}}$$

$$+ \frac{X_n}{3}$$

(I.20)

Similarly, one may list the indices of $\lambda$ as $m = (3, 9), (4, 10)$. For example, $(3, 9)$ is a set of two indices, representing the $\pm$ cases in the solution. Then $n = 1, 2$ represent the indices of a set of solutions. For example, $\lambda_{3,9}$ used $X_1, Y_1$, and $Z_1$.

$$\lambda_m = -\frac{1}{6\sqrt[3]{2}} \left( 1 \pm i\sqrt{3} \right)$$

$$+ \frac{\sqrt[3]{2X_n^3 + 3\sqrt{3}X_n^3Z_n - X_n^2Y_n^2 + 18X_nY_nZ_n - 4Y_n^3 + 27Z_n^2 + 9X_nY_n + 27Z_n}}{3 \times 2\sqrt[3]{2}}$$

$$- \frac{(1 \mp i\sqrt{3}) (-X_n^2 - 3Y_n)}{3 \times 2\sqrt[3]{2}}$$

$$+ \frac{X_n}{3}$$

(I.21)

Here, $\lambda_{3,6,9}$ is using $X_1, Y_1,$ and $Z_1$. $\lambda_{4,7,10}$ is using $X_2, Y_2,$ and $Z_2$. 

192
Due to the size of the matrix, define

\[ A_1 = \mu_1 + \Omega_{1, -\frac{1}{2}}^{\frac{1}{2}} - \lambda, \quad A_2 = \mu_2 + \Omega_{1, \frac{3}{2}}^{\frac{1}{2}} - \lambda, \quad A_3 = \mu_3 + \Omega_{1, \frac{3}{2}}^{\frac{1}{2}} - \lambda \]
\[ A_4 = \mu_4 + \Omega_{1, -\frac{1}{2}}^{\frac{1}{2}} - \lambda, \quad A_5 = \mu_5 + \Omega_{1\cdot \frac{3}{2} - \frac{3}{2}}^{\frac{1}{2}} - \lambda, \quad A_6 = \mu_6 + \Omega_{1\cdot \frac{3}{2} - \frac{3}{2}}^{\frac{1}{2}} - \lambda \]
\[ A_7 = \mu_7 + \Omega_{0, \frac{1}{2}}^{\frac{1}{2}} - \lambda, \quad A_8 = \mu_8 + \Omega_{0\cdot \frac{1}{2} - \frac{3}{2}}^{\frac{1}{2}} - \lambda, \quad A_9 = \mu_9 + \Omega_{0\cdot \frac{1}{2} - \frac{3}{2}}^{\frac{1}{2}} - \lambda \]
\[ A_{10} = \mu_9 + \Omega_{0\cdot \frac{1}{2} - \frac{3}{2}}^{\frac{1}{2}} - \lambda, \quad A_{11} = \mu_8 + \Omega_{0\cdot \frac{1}{2} - \frac{3}{2}}^{\frac{1}{2}} - \lambda, \quad A_{12} = \mu_7 + \Omega_{0\cdot \frac{1}{2} - \frac{3}{2}}^{\frac{1}{2}} - \lambda \]
\[ A_{13} = \mu_6 + \Omega_{-1\cdot \frac{1}{2} - \frac{3}{2}}^{\frac{1}{2}} - \lambda, \quad A_{14} = \mu_5 + \Omega_{-1\cdot \frac{1}{2} - \frac{3}{2}}^{\frac{1}{2}} - \lambda, \quad A_{15} = \mu_4 + \Omega_{-1\cdot \frac{1}{2} - \frac{3}{2}}^{\frac{1}{2}} - \lambda \]
\[ A_{16} = \mu_3 + \Omega_{-1\cdot \frac{1}{2} - \frac{3}{2}}^{\frac{1}{2}} - \lambda, \quad A_{17} = \mu_2 + \Omega_{-1\cdot \frac{1}{2} - \frac{3}{2}}^{\frac{1}{2}} - \lambda, \quad A_{18} = \mu_1 + \Omega_{-1\cdot \frac{1}{2} - \frac{3}{2}}^{\frac{1}{2}} - \lambda \]

For simplification all terms inside the original matrix are represented by single terms, and the matrix element blank if its corresponding value is zero. The original matrix can be color coded and written as

Figure I.8: I=1 and J=5/2 Original Magnetic Dipole and Electric Quadrupole Moment Matrix
Similar to the $I = 1$ and $J = 3/2$ case, processed to matrix reduction obtains,

![Matrix Image]

Figure I.9: The Matrices After the First Reduction from the Original Rank 18 Matrix

In the case of the left a rank 2 matrix, it could determine the values for $\lambda_{1,18}$

$$\lambda_{1,18} = \mu_1 + \Omega_{\pm 1, \pm \frac{5}{2}}^{\pm \frac{5}{2}}$$  \hspace{1cm} (I.23)

The remaining rank 16 matrix can be reduced to smaller size matrices, by following processes
Figure I.10: The Process of Transforming the Rank 16 Matrix for Matrix Reduction

Similar to the $I = 1$ and $J = 3/2$ case, the matrix transformation follows the same rules for changing the rows and columns. The final form can be written as
Figure I.11: The Rank 16 Matrix After Transformation

Basically, the rank 16 matrix can be transformed to 2 rank 2 matrices and 4 rank 3 matrices. The determinant of the first (upper left) rank 2 matrix determinant can be written as

\[
\begin{vmatrix}
A_2 & \Gamma_1 \\
\Gamma_1 & A_7
\end{vmatrix} = A_2 A_7 - \Gamma_1^2
\]

\[
= \left( \mu_2 + \Omega_{1,\frac{1}{2}}^{\frac{1}{2}} - \lambda \right) \left( \mu_7 + \Omega_{1,-\frac{1}{2}}^{\frac{1}{2}} - \lambda \right) - \Gamma_1^2
\]

\[
= \lambda^2 - \lambda \left( \mu_2 + \mu_7 + \Omega_{1,\frac{1}{2}}^{\frac{1}{2}} + \Omega_{1,-\frac{1}{2}}^{\frac{1}{2}} \right)
\]

\[
+ \mu_2 \mu_7 + \mu_2 \Omega_{1,-\frac{1}{2}}^{\frac{1}{2}} + \mu_7 \Omega_{1,\frac{1}{2}}^{\frac{1}{2}} + \Omega_{1,\frac{1}{2}}^{\frac{1}{2}} \Omega_{1,-\frac{1}{2}}^{\frac{1}{2}}
\] (I.24)
Therefore,

\[
\lambda_{2,7} = \frac{(\mu_2 + \mu_7 + \Omega_{1,\frac{1}{2}}^{1,\frac{5}{2}} + \Omega_{1,-\frac{1}{2}}^{1,\frac{5}{2}})}{2} + 4 \left(\mu_2 \mu_7 + \mu_2 \Omega_{1,-\frac{1}{2}}^{1,\frac{5}{2}} + \mu_7 \Omega_{1,\frac{1}{2}}^{1,\frac{5}{2}} + \Omega_{1,\frac{1}{2}}^{1,\frac{5}{2}} \Omega_{1,-\frac{1}{2}}^{1,\frac{5}{2}}\right)
\]

(I.25)

The second (lower right) rank 2 matrix determinant can be written as

\[
\begin{vmatrix}
A_{12} & \Gamma_1 \\
\Gamma_1 & A_{17}
\end{vmatrix} = A_{12} A_{17} - \Gamma_1^2 = \left(\mu_7 + \Omega_{0,-\frac{1}{2}}^{1,\frac{5}{2}} - \lambda\right) \left(\mu_2 + \Omega_{-1,-\frac{1}{2}}^{1,\frac{5}{2}} - \lambda\right) - \Gamma_1^2
\]

\[
= \lambda^2 - \lambda \left(\mu_2 + \mu_7 + \Omega_{-1,-\frac{1}{2}}^{1,\frac{5}{2}} + \Omega_{0,-\frac{1}{2}}^{1,\frac{5}{2}}\right)
\]

\[
+ \mu_2 \mu_7 + \mu_2 \Omega_{0,-\frac{1}{2}}^{1,\frac{5}{2}} + \mu_7 \Omega_{-1,-\frac{1}{2}}^{1,\frac{5}{2}} + \Omega_{0,-\frac{1}{2}}^{1,\frac{5}{2}} \Omega_{-1,-\frac{1}{2}}^{1,\frac{5}{2}}
\]

(I.26)

Therefore,

\[
\lambda_{12,17} = \frac{(\mu_2 + \mu_7 + \Omega_{-1,-\frac{1}{2}}^{1,\frac{5}{2}} + \Omega_{0,-\frac{1}{2}}^{1,\frac{5}{2}})}{2} + 4 \left(\mu_2 \mu_7 + \mu_2 \Omega_{0,-\frac{1}{2}}^{1,\frac{5}{2}} + \mu_7 \Omega_{-1,-\frac{1}{2}}^{1,\frac{5}{2}} + \Omega_{0,-\frac{1}{2}}^{1,\frac{5}{2}} \Omega_{-1,-\frac{1}{2}}^{1,\frac{5}{2}}\right)
\]

(I.27)

The determinant of the uppermost of the four rank 3 matrices determinant can be written as
Therefore, equation I.28 has the cubic form 

\[-\lambda^3 + X_3\lambda^2 + Y_3\lambda + Z_3 = 0,\]

where

\[
\begin{align*}
X_3 &= \Omega_{1/2}^{\frac{1}{2}} + \Omega_{1,-1/2}^{\frac{1}{2}} + \Omega_{1,-1/2}^{\frac{1}{2}} + \mu_4 + \mu_5 + \mu_9 \\
Y_3 &= \Gamma_3^2 + \Gamma_3^2 - \Omega_{1/2}^{\frac{1}{2}} \Omega_{1,-1/2}^{\frac{1}{2}} - \Omega_{0,3}^{\frac{1}{2}} \Omega_{1,2}^{\frac{1}{2}} - \Omega_{0,3}^{\frac{1}{2}} \Omega_{1,2}^{\frac{1}{2}} - \Omega_{0,3}^{\frac{1}{2}} \mu_4 - \Omega_{1,2}^{\frac{1}{2}} \mu_5 - \Omega_{1,2}^{\frac{1}{2}} \Omega_{1,2}^{\frac{1}{2}} \\
Z_3 &= \mu_4\mu_5\mu_9 - \Gamma_2^2 \Omega_{0,3}^{\frac{1}{2}} - \Gamma_2^2 \mu_9 + \Gamma_2 \Gamma_3^2 \delta_2 - \Gamma_3 \Omega_{1,2}^{\frac{1}{2}} - \Gamma_2^2 \mu_5 + \Omega_{1,2}^{\frac{1}{2}} \Omega_{1,2}^{\frac{1}{2}} \Omega_{1,2}^{\frac{1}{2}} \Omega_{1,2}^{\frac{1}{2}} \mu_4 + \Gamma_2 \Omega_{1,2}^{\frac{1}{2}} \Omega_{1,2}^{\frac{1}{2}} \mu_4 + \Omega_{1,2}^{\frac{1}{2}} \mu_5 \mu_9 + \delta_2 \mu_9
\end{align*}
\]
The determinant of the second rank 3 matrix (middle left) can be written,

\[
\begin{vmatrix}
A_3 & \Gamma_2 & \delta_1 \\
\Gamma_2 & A_8 & \Gamma_1 \\
\delta_1 & \Gamma_1 & A_{13}
\end{vmatrix} = A_3 \begin{vmatrix}
A_8 & \Gamma_1 \\
\Gamma_1 & A_{13}
\end{vmatrix} - \Gamma_2 \begin{vmatrix}
\Gamma_2 & \delta_1 \\
\delta_1 & A_{13}
\end{vmatrix} + \delta_1 \begin{vmatrix}
\Gamma_2 & \delta_1 \\
\delta_1 & A_{13}
\end{vmatrix}
\]

\[
= A_3 A_8 A_{13} - A_3 \Gamma_1^2 - A_{13} \Gamma_2^2 + \Gamma_1 \Gamma_2 \delta_1 + \Gamma_1 \Gamma_2 \delta_1 - A_8 \delta_1^2
\]

\[
= \left( \mu_3 + \Omega_{1,2}^{1,5} - \lambda \right) \left( \mu_8 + \Omega_{0,2}^{1,5} - \lambda \right) \left( \mu_6 + \Omega_{-1,-2}^{1,5} - \lambda \right)
\]

\[
- \left( \mu_3 + \Omega_{1,2}^{1,5} - \lambda \right) \delta_1^2
\]

\[
- \lambda^3 + \lambda^2 \left( \Omega_{0,2}^{1,5} + \Omega_{1,2}^{1,5} + \Omega_{-1,-2}^{1,5} + \mu_3 + \mu_6 + \mu_8 \right) + \lambda \left( \Gamma_1^2 - \Omega_{0,2}^{1,5} \Omega_{1,2}^{1,5} \right)
\]

\[
- \Omega_{-1,-2}^{1,5} \mu_3 - \Omega_{-1,-2}^{1,5} \mu_8 + \delta_1^2 - \mu_3 \mu_6 - \mu_3 \mu_8 - \mu_6 \mu_8
\]

\[
- \Gamma_1^2 \Omega_{1,2}^{1,5} - \Gamma_1^2 \mu_3 + 2 \Gamma_1 \Gamma_2 \delta_1 + \Omega_{0,2}^{1,5} \Omega_{1,2}^{1,5} \Omega_{-1,-2}^{1,5} + \Omega_{0,2}^{1,5} \Omega_{1,2}^{1,5} \mu_6
\]

\[
+ \Omega_{0,2}^{1,5} \Omega_{-1,-2}^{1,5} \mu_3 - \Omega_{0,2}^{1,5} \delta_1^2 + \Omega_{0,2}^{1,5} \mu_3 \mu_6 + \Omega_{1,2}^{1,5} \Omega_{-1,-2}^{1,5} \mu_8 + \Omega_{1,2}^{1,5} \mu_6 \mu_8
\]

\[
+ \Omega_{-1,-2}^{1,5} \mu_3 \mu_8 - \delta_1^2 \mu_8
\]

(I.30)
Therefore, the equation I.30 matches the form $-\lambda^3 + X_4\lambda^2 + Y_4\lambda + Z_4 = 0$.

$$X_4 = \Omega^{\frac{1}{2}}_0 + \Omega^{\frac{1}{2}}_1 + \Omega^{\frac{1}{2}}_{-1, \frac{1}{2}} + \mu_3 + \mu_6 + \mu_8$$

$$Y_4 = \Gamma^2_1 - \Omega^{\frac{1}{2}}_0 + \Omega^{\frac{1}{2}}_1 - \Omega^{\frac{1}{2}}_0\mu_3 - \Omega^{\frac{1}{2}}_0\mu_6 - \Omega^{\frac{1}{2}}_1\mu_3 - \Omega^{\frac{1}{2}}_1\mu_6 - \Omega^{\frac{1}{2}}_{-1, \frac{1}{2}}\mu_8 - \delta^2_1 - \mu_3\mu_6 - \mu_3\mu_8 - \mu_6\mu_8$$

$$Z_4 = \mu_3\mu_6\mu_8 - \Gamma^2_1\Omega^{\frac{1}{2}}_1 - 2\Gamma_1\Gamma_2\delta_1 + \Omega^{\frac{1}{2}}_0\Omega^{\frac{1}{2}}_1 + \Omega^{\frac{1}{2}}_0\Omega^{\frac{1}{2}}_{-1, \frac{1}{2}} - \Omega^{\frac{1}{2}}_0\mu_3 + \Omega^{\frac{1}{2}}_0\mu_6 + \Omega^{\frac{1}{2}}_1\mu_3 + \Omega^{\frac{1}{2}}_1\mu_6 + \Omega^{\frac{1}{2}}_{-1, \frac{1}{2}}\mu_8 + \mu^2 + \Gamma^2_3\mu_3\mu_6$$

$$+\Omega^{\frac{1}{2}}_{-1, \frac{1}{2}}\mu_3 - \delta^2_1\mu_8$$

(I.31)

The determinant of the third rank 3 matrix (middle right) can be written,

$$| A_{10} \quad \Gamma_2 \quad -\Gamma_3 | = A_{10} | A_{15} \quad -\delta_2 | = A_{10} | A_{15} \quad -\delta_2 | = A_{10} | A_{15} \quad -\delta_2 |$$

(I.32)
Therefore, the equation I.32 matches the form $-\lambda^3 + X_5\lambda^2 + Y_5\lambda + Z_5 = 0$.

\begin{align*}
X_5 &= \Omega_{0,-\frac{1}{2}}^{1,\frac{1}{2}} + \Omega_{1,-\frac{3}{2}}^{1,\frac{1}{2}} + \Omega_{-\frac{1}{2},\frac{1}{2}}^{1,\frac{1}{2}} + \mu_4 + \mu_5 + \mu_9 \\
Y_5 &= \Gamma_{-\frac{1}{2}}^2 - \Gamma_{-\frac{3}{2}}^2 - \Omega_{0,-\frac{1}{2}}^{1,\frac{3}{2}} \Omega_{1,-\frac{1}{2}}^{1,\frac{3}{2}} - \Omega_{0,-\frac{1}{2}}^{1,\frac{1}{2}} \Omega_{-\frac{1}{2},\frac{1}{2}}^{1,\frac{1}{2}} - \Omega_{0,-\frac{1}{2}}^{1,\frac{1}{2}} \mu_4 - \Omega_{0,-\frac{1}{2}}^{1,\frac{1}{2}} \mu_5 - \Omega_{-\frac{1}{2},\frac{1}{2}}^{1,\frac{1}{2}} \Omega_{-1,-\frac{1}{2}}^{1,\frac{1}{2}} \\
&\quad - \Omega_{-\frac{1}{2},\frac{1}{2}}^{1,\frac{1}{2}} \mu_4 - \Omega_{-\frac{1}{2},\frac{1}{2}}^{1,\frac{1}{2}} \mu_9 - \Omega_{-\frac{1}{2},\frac{1}{2}}^{1,\frac{1}{2}} \mu_5 - \Omega_{-\frac{1}{2},\frac{1}{2}}^{1,\frac{1}{2}} \mu_9 - \mu_4 \mu_5 - \mu_4 \mu_9 - \mu_5 \mu_9 \\
Z_5 &= \mu_4 \mu_5 \mu_9 - \Gamma_{-\frac{1}{2}}^2 \Omega_{-1,-\frac{1}{2}}^{1,\frac{3}{2}} + \Gamma_{-\frac{3}{2}}^2 \mu_4 + \Gamma_{3,-\frac{1}{2}}^2 \Omega_{1,-\frac{1}{2}}^{1,\frac{3}{2}} + \Gamma_{\frac{1}{2},\frac{1}{2}}^2 \mu_5 + \Omega_{-\frac{1}{2},\frac{1}{2}}^{1,\frac{1}{2}} \Omega_{1,-\frac{3}{2}}^{1,\frac{1}{2}} \Omega_{-1,-\frac{1}{2}}^{1,\frac{1}{2}} \\
&\quad + \Omega_{-\frac{1}{2},\frac{1}{2}}^{1,\frac{1}{2}} \Omega_{1,-\frac{3}{2}}^{1,\frac{1}{2}} \mu_4 + \Omega_{0,-\frac{1}{2}}^{1,\frac{3}{2}} \Omega_{-1,-\frac{1}{2}}^{1,\frac{3}{2}} \mu_5 + \Omega_{0,-\frac{1}{2}}^{1,\frac{1}{2}} \mu_4 \mu_5 + \Omega_{1,-\frac{3}{2}}^{1,\frac{1}{2}} \Omega_{-1,-\frac{1}{2}}^{1,\frac{1}{2}} \mu_9 \\
&\quad + \Omega_{1,-\frac{1}{2}}^{1,\frac{1}{2}} \mu_4 \mu_9 + \Omega_{-1,\frac{1}{2}}^{1,\frac{1}{2}} \mu_5 \mu_9
\end{align*}
The determinant of the last rank 3 matrix (bottom right) can be written,

\[
\begin{vmatrix}
A_{11} & \Gamma_1 & -\Gamma_2 \\
\Gamma_1 & A_6 & -\delta_1 \\
-\Gamma_2 & -\delta_1 & A_{16}
\end{vmatrix} = A_{11} \begin{vmatrix} A_6 & -\delta_1 \\ -\delta_1 & A_{16} \end{vmatrix} - \Gamma_1 \begin{vmatrix} \Gamma_1 & -\Gamma_2 \\ -\delta_1 & A_{16} \end{vmatrix} - \Gamma_2 \begin{vmatrix} \Gamma_1 & -\Gamma_2 \\ A_6 & -\delta_1 \end{vmatrix}
\]

\[
= A_6 A_{11} A_{16} - A_1 \delta_1^2 - \Gamma_1^2 A_{16} + \Gamma_1 \Gamma_2 \delta_1 + \Gamma_1 \Gamma_2 \delta_1 - \Gamma_2^2 A_6
\]

\[
= \left( \mu_6 + \Omega_{0,-1/2}^{1/2} - \lambda \right) \left( \mu_8 + \Omega_{0,-3/2}^{1/2} - \lambda \right) \left( \mu_3 + \Omega_{-1,-1/2}^{1/2} - \lambda \right)
\]

\[
- \left( \mu_8 + \Omega_{0,-3/2}^{1/2} - \lambda \right) \delta_1^2 - \Gamma_2^2 \left( \mu_3 + \Omega_{-1,-1/2}^{1/2} - \lambda \right) + \Gamma_1 \Gamma_2 \delta_1 + \Gamma_1 \Gamma_2 \delta_1
\]

\[
- \Gamma_2^2 \left( \mu_6 + \Omega_{1,-1/2}^{1/2} - \lambda \right)
\]

\[
= - \lambda^3 + \lambda^2 \left( \Omega_{0,-1/2}^{1/2} + \Omega_{-1,-1/2}^{1/2} + \Omega_{-1,-3/2}^{1/2} + \mu_3 + \mu_6 + \mu_8 \right) + \lambda \Gamma_2^2 + \Gamma_2^2
\]

\[
- \Omega_{0,-1/2}^{1/2} - \Omega_{0,-3/2}^{1/2} \Omega_{-1,-1/2}^{1/2} - \Omega_{0,-3/2}^{1/2} \mu_3 - \Omega_{0,-3/2}^{1/2} \mu_6 - \Omega_{0,-3/2}^{1/2} \Omega_{-1,-1/2}^{1/2}
\]

\[
- \Omega_{1,-1/2}^{1/2} \mu_3 - \Omega_{1,-1/2}^{1/2} \mu_8 - \Omega_{-1,-1/2}^{1/2} \mu_6 - \Omega_{0,-1/2}^{1/2} \delta_1^2 - \mu_3 \mu_6 - \mu_3 \mu_8
\]

\[
- \mu_6 \mu_8 + \mu_3 \mu_6 \mu_8 - \Gamma_1^2 \Omega_{-1,-1/2}^{1/2} - \Gamma_1^2 \Omega_{-1/2}^{1/2} - \Gamma_1^2 \Omega_{-1/2}^{1/2} - \Gamma_1^2 \Omega_{-1/2}^{1/2}
\]

\[
+ \Omega_{0,-1/2}^{1/2} \Omega_{-1,-1/2}^{1/2} + \Omega_{0,-3/2}^{1/2} \Omega_{1,-1/2}^{1/2} \mu_3 + \Omega_{0,-3/2}^{1/2} \Omega_{-1,-1/2}^{1/2} \mu_6 - \Omega_{0,-3/2}^{1/2} \delta_1^2
\]

\[
+ \Omega_{0,-1/2}^{1/2} \mu_3 \mu_6 + \Omega_{1,-1/2}^{1/2} \mu_8 + \Omega_{1,-1/2}^{1/2} \mu_3 \mu_8 + \Omega_{1,-1/2}^{1/2} \mu_6 \mu_8 - \delta_1^2 \mu_8
\]

(I.34)

Therefore, the equation I.34 matches the form 

\[-\lambda^3 + X_6 \lambda^2 + Y_6 \lambda + Z_6 = 0.\]

\[
X_6 = \Omega_{0,-1/2}^{1/2} + \Omega_{1,-1/2}^{1/2} + \Omega_{-1,-3/2}^{1/2} + \mu_3 + \mu_6 + \mu_8
\]

\[
Y_6 = \Gamma_1^2 - \Gamma_2^2 - \Omega_{0,-1/2}^{1/2} \Omega_{1,-1/2}^{1/2} - \Omega_{0,-3/2}^{1/2} \Omega_{-1,-1/2}^{1/2} - \Omega_{0,-3/2}^{1/2} \mu_3 - \Omega_{0,-3/2}^{1/2} \mu_6 - \Omega_{0,-3/2}^{1/2} \Omega_{-1,-1/2}^{1/2}
\]

\[
- \Omega_{1,-1/2}^{1/2} \mu_3 - \Omega_{1,-1/2}^{1/2} \mu_8 - \Omega_{-1,-1/2}^{1/2} \mu_6 - \Omega_{0,-1/2}^{1/2} \delta_1^2 - \mu_3 \mu_6 - \mu_3 \mu_8 - \mu_6 \mu_8
\]

(I.35)

\[
Z_6 = \mu_3 \mu_6 \mu_8 - \Gamma_2^2 \Omega_{1,-1/2}^{1/2} - \Gamma_2^2 \mu_3 + 2 \Gamma_1 \Gamma_2 \delta_1 - \Gamma_2^2 \Omega_{1,-1/2}^{1/2} - \Gamma_2^2 \mu_6
\]

\[
+ \Omega_{0,-1/2}^{1/2} \Omega_{1,-1/2}^{1/2} + \Omega_{0,-3/2}^{1/2} \Omega_{1,-1/2}^{1/2} \mu_3 + \Omega_{0,-3/2}^{1/2} \Omega_{1,-1/2}^{1/2} \mu_6 - \Omega_{0,-3/2}^{1/2} \delta_1^2
\]

\[
+ \Omega_{0,-1/2}^{1/2} \mu_3 \mu_6 + \Omega_{1,-1/2}^{1/2} \mu_8 + \Omega_{1,-1/2}^{1/2} \mu_3 \mu_8 + \Omega_{1,-1/2}^{1/2} \mu_6 \mu_8 - \delta_1^2 \mu_8
\]
One may list the four indices of $\lambda$ as $m = 9, 8, 5, 6$ and $n = 3, 4, 5, 6$, respectively. For example, $\lambda_9$ employs $X_3, Y_3$, and $Z_3$. Therefore, the solutions of $\lambda$ can be written as

$$\lambda_m = \frac{3\sqrt[3]{2} X_n^3 + 3\sqrt[3]{3} \sqrt{4X_n^3 Z_n - X_n^2 Y_n^2 + 18X_n Y_n Z_n - 4Y_n^3 + 27Z_n^2 + 9X_n Y_n + 27Z_n}}{3\sqrt[3]{2}} - \frac{3\sqrt[3]{2} X_n^3 + 3\sqrt[3]{3} \sqrt{4X_n^3 Z_n - X_n^2 Y_n^2 + 18X_n Y_n Z_n - 4Y_n^3 + 27Z_n^2 + 9X_n Y_n + 27Z_n}}{3\sqrt[3]{2} (-X_n - 3Y_n)}$$

$$+ \frac{X_n}{3}$$

(I.36)

Similarly, one may list the indices of $\lambda$ as $m = (4, 14), (3, 13), (10, 15), (11, 16)$. For example, $(4, 14)$ is a set of indices, representing the $\pm$ cases in the solution. Then $n = 3, 4, 5, 6$ represents the indices of a set of solutions. For example, $\lambda_{4,14}$ employs $X_3, Y_3, Z_3$.

$$\lambda_m = -\frac{1}{6\sqrt{2}} \left( 1 \pm i\sqrt{3} \right)$$

$$+ \sqrt[3]{2} X_n^3 + 3\sqrt[3]{3} \sqrt{4X_n^3 Z_n - X_n^2 Y_n^2 + 18X_n Y_n Z_n - 4Y_n^3 + 27Z_n^2 + 9X_n Y_n + 27Z_n}$$

$$+ \frac{1}{3} \left( 1 \mp i\sqrt{3} \right) (-X_n - 3Y_n)$$

$$+ \frac{X_n}{3}$$

(I.37)

In here, $\lambda_{4,9,14}$ employs $X_3, Y_3$, and $Z_3$; $\lambda_{3,8,13}$ employs $X_4, Y_4$, and $Z_4$; $\lambda_{10,5,15}$ employs $X_5, Y_5$, and $Z_5$; and $\lambda_{11,6,16}$ employs $X_6, Y_6$, and $Z_6$. 

203
LIST OF REFERENCES


