LIPMAN, ADAM SCOTT. Development of Simulations Framework to Study Trapped Particle Spin Dynamics Regarding the Search for an nEDM. (Under the direction of Robert Golub and Paul Huffman.)

Simulations to study ultracold neutrons and $^3$He in a trap are crucial for appropriate measurement of a neutron electric dipole moment. At record sensitivity, the nEDM experiment at SNS will aim to put an upper limit on an nEDM of $1.6 \times 10^{-28}$ e·cm. This paper examines how to benchmark ComSol to properly study spin dynamics; the use of a fourth order Runge-Kutta solver for spin dressing which showed the existence of anomalous frequencies that will affect the $\vec{\sigma}_3 \cdot \vec{\sigma}_n$ scintillation rate; the modulation of the dressing field about the critical dressing parameter and the correction needed to sufficiently offset effects from a $^3$He pseudomagnetic field.
Development of Simulations Framework to Study Trapped Particle Spin Dynamics Regarding the Search for an nEDM

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BIOGRAPHY

Born in Livingston, NJ, I became interested in physics during high school where I took physics honors and then AP physics C. I excelled in my physics major at Rutgers University and chose to continue pursuing physics at NC State University. At NCSU, I continued my research in Nuclear Physics and eventually settled into a theory position examining systematic effects in the nEDM experiment.
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1.1 What are electric dipole moments?

An electric dipole moment (EDM) is a measure of overall polarity for a particle, molecule or system. In the simplest case, an EDM $d$ is created from the separation of a positive and negative charge

$$\vec{d} = e \vec{l} \cdot \text{cm},$$

where this applies to two particles of charge $\pm e$ separated by a distance $l$. $\vec{l}$ points from the negative to the positive charge. For a distribution of charges described by $\rho$, an EDM is

$$\vec{d} = \int d^3 \rho \vec{x} = d \hat{S},$$

where the integral is over volume and the last expression indicates that an EDM always points along the spin vector. In an electric field $\vec{E}$, the EDM is subject to a force and a torque that tends to align $\vec{l}$ with the field. The potential energy and torque, analogous to magnetic dipole moments in magnetic fields, is

$$U = -\vec{d} \cdot \vec{E}, \quad \vec{\tau} = \vec{d} \times \vec{E}.$$  

The Hamiltonian of a particle with an EDM and magnetic dipole moment $\mu$ in a magnetic and electric field is

$$H = -\mu \cdot \vec{B} - \vec{d} \cdot \vec{E}.$$


1.2 Symmetry Violations

Symmetries in physics have been an important topic of research for decades as discussed in [Gol94]. Symmetries are directly related to conservation laws. Asymmetries perplex physicists because their source often requires new theories and physics. Two known symmetries are how some process performed at one point in space or time will be exactly reproducible at some other point in space or time given everything else is equal. Through these symmetries and their expressions as operators, it can be shown they lead to the conservation of momentum and energy. Another critical symmetry is rotation - some process will have the same result before and after a rotation through some angle. This leads to the conservation of angular momentum.

Parity (P), time-reversal (T) and charge conjugation (C) are three symmetries that only recent (second half of 20th century) experiments provided evidence for their violations. However, the combination of CPT is a symmetry that must hold for any Lorentz invariant theory with a Hermitian Hamiltonian. The search for an EDM of an elementary particle is such a sought after experiment because it would provide direct evidence for T and CP violation (which conserves CPT). Hence, finding an nEDM and where its value lies, ie. $10^{-28} \text{e-cm}$, will shed light on other observations and phenomena that violate CP and T.

Parity conservation means a reflection of spatial coordinates about the origin causes no change to a system or its measurable quantities. Time reversal conservation means processes are symmetric whether time moves forward or backward. Finally, charge conjugation symmetry occurs when flipping the sign of all quantum numbers has no affect on the observables of the system. Then, CPT symmetry says a mirror image of our universe behaves under the exact laws as the initial universe. While CPT symmetry has yet to be dis-proven, it has now been shown through experiments starting in the 1950s that C and P can be violated individually. Then CP was violated. It’s very hard to experimentally test T conservation but when CP violation exists, there are thought experiments that will also lead to T violation.

1.2.1 Parity Invariance

In classical and quantum mechanics, the parity operator transforms quantities in different manners. In classical mechanics, parity operates as

\[ P x^i = -x^i \]
\[ P p^i = -p^i. \]  \hspace{1cm} (1.5) \hspace{1cm} (1.6)

Whereas in quantum mechanics, parity operates on a state as

\[ \Pi |x\rangle = |-x\rangle \]
\[ \Pi |p\rangle = |p\rangle \] \hspace{1cm} (1.7) \hspace{1cm} (1.8)
and
\[ \Pi |\psi\rangle = \Pi \int_{-\infty}^{\infty} |x\rangle \langle x| \psi \rangle dx = \int_{-\infty}^{\infty} |x\rangle \langle x| \psi \rangle dx = \int_{-\infty}^{\infty} |x\rangle \langle x'| \psi \rangle dx', \]
\[ \langle x| \psi \rangle = \psi(x), \langle x| \Pi |\psi\rangle = \psi(-x). \] (1.9)

So in classical mechanics, the parity operator reflects spatial coordinates about the origin. Equivalently, in quantum mechanics, \(\psi(-x)\) is the mirror image of \(\psi(x)\) about the origin.

Parity acts on an operator such as \(X\) like \(\Pi X \Pi^* = -X\). A parity invariant Hamiltonian obeys the following
\[ \Pi^* H(X, P) \Pi = H(-X, -P) = H(X, P); \quad [\Pi, H] = 0. \] (1.10)

Given the commutator between the parity operator and \(H\) is zero and with the absence of degeneracy, it can be shown [Gol94] that the eigenfunctions of the Hamiltonian are eigenstates of the parity operator. Since the expected Hamiltonian, \(H = -\vec{d} \cdot \vec{E}\), is Hermitian and assuming its eigenvalues are non-degenerate, I can use properties of a self-adjoint operator to show distinct eigenfunctions are orthogonal
\[ \langle \psi_1| H \psi_2 \rangle = E_2 \langle \psi_1| \psi_2 \rangle = \langle H^* \psi_1| \psi_2 \rangle = \langle H \psi_1| \psi_2 \rangle = E_1^* \langle \psi_1| \psi_2 \rangle = E_1 \langle \psi_1| \psi_2 \rangle; \] (1.11)
\[ \langle \psi_1| \psi_2 \rangle = 0. \] (1.12)

From there, I calculate the expectation value of the parity-Hamiltonian commutator
\[ \int \psi_j^* [\Pi H - H \Pi] \psi_j d\nu = (E_j - E_i) \int \psi_j^* \Pi \psi_j d\nu = 0. \] (1.13)

This means \(\Pi\) is a symmetry of the wavefunctions since any change to \(\psi_j\) would render the expectation value non-zero. However, in regards to an nEDM, the eigenstates of the parity conserving Hamiltonian, \(H = -\vec{d}_n \cdot \vec{E}\), must conserve parity (the vectors \(\vec{d}_n\) and \(\vec{E}\) have parity eigenvalues of -1). But if the eigenfunctions are eigenstates of parity, the expectation value of \(\vec{d}_n\) is zero which I will show. Since the neutron does not have a degenerate ground state, \(\psi_i\)'s are eigenstates of the parity operator with eigenvalues of \(\pm 1\) since \(H\) commutes with \(\Pi\). The expectation value is
\[ \langle \vec{d} \rangle = \int \psi^* \vec{d} \psi d\nu, \] (1.14)
then with applying a parity operator
\[ \Pi \langle \vec{d} \rangle = \int (\pm \psi^*) (-\vec{d})(\pm \psi) d\nu = -\langle \vec{d} \rangle. \] (1.15)

For the expectation value of \(\vec{d}\) to be non-zero, \(\psi\) must be of the parity-violating form. What this means is our Hamiltonian is incorrect since it conserves parity and commutes with it. A need for parity violating eigenstates leads us to believe there's something we're missing in the Hamiltonian. The expectation value of \(\vec{d}\) can only be non-zero if \(\psi\) takes the parity violating form: \(\psi = a \psi_+ + b \psi_-\) where the + and -
correspond to +1 and -1 parity eigenvalues. This will make the integral in Equation 1.13 invariant under parity.

Physicists Lee and Yang started to question parity invariance in the 1950s when there was a particle with two different decay mechanisms with products having total parity of opposite sign [Gol94]. It was called the $\tau - \theta$ puzzle and the puzzle was concerning the $K^+$ particle. The decay modes were

$$
\begin{align*}
\tau^+ &\longrightarrow 2\pi^+ + \pi^-,
\tau^+ &\longrightarrow \pi^+ + 2\pi^0 \\
\theta^+ &\longrightarrow \pi^+ + \pi^0.
\end{align*}
$$

Both $\tau^+$ and $\theta^+$ had the same masses, production rates and lifetimes leading scientists to believe they were the same particle. However, Equation 1.16's products have a parity of -1 while Equation 1.17's parity is +1 (given both decays result in pi mesons of $J=0$). Either the conservation of angular momentum or parity conservation is being violated. The former was very well established so Lee and Yang developed an idea for an experiment to test whether there's spatial symmetry in $\beta$ decay.

In 1956, Lee and Yang realized that there was plenty of parity invariance in the strong and electromagnetic interactions but not much for the weak interaction. From there, Wu devised a weak interaction test from the decay of Cobalt-60. The spins of $^{60}$Co were all aligned in say the $+z$ direction so that the direction of electrons from beta decay could be recorded. The electrons’ momentum were opposite of the Cobalt's spin. However, when the Cobalt was set up with their spin in the $-z$ direction, the electrons had momentum aligned with the spin! This was the first experimental violation of parity. This revelation led to further experiments, specifically those involving neutrinos. A spin 1/2 particle can have a helicity of +1/2 or -1/2 corresponding to right-handedness and left-handedness respectively. What was discovered was that neutrinos are left-handed and anti-neutrinos are right-handed. The experiment was measuring the handedness of a muon in the decay of a pion: $\pi^- \longrightarrow \mu^- + \bar{\nu}_\mu$. It was shown that the handedness of the muon changed when the charge of the pion changes and so does the handedness of the neutrino. So neutrinos were left handed and anti-neutrinos right handed. From there, scientists began to believe the mirror image of the neutrino does not exist. However, a right-handed neutrino must exist.

### 1.2.2 Charge Conjugation

Charge conjugation changes more than just the charge of a particle. It changes the sign of all internal quantum numbers, transforming the particle to its anti-particle: $C \ket{p} = \ket{\bar{p}}$. As with the parity operator, C has eigenvalues of ±1. However, most particles are not eigenstates of C since in order to be one, a particle has to be its own anti-particle. Evidence has shown charge conjugation is conserved in the strong and electromagnetic interactions while violated in the weak interaction. When C is applied to a neutrino (anti-neutrino), a right-handed neutrino (left-handed anti-neutrino) is the result. As we have never observed such particles, charge conjugated neutrino processes are not physical processes.
1.2.3 CP

After observing P and C violations, it seemed that a mirror image should be more than an inversion of spatial coordinates. A mirror image should be an inversion and a charge conjugation. So a right-handed electron being transformed to a left-handed positron would occur when applying CP to the former. It was then thought that C and P violation made sense as the operation of CP has otherwise been conserved.

Further investigation into the conservation of CP [Gol94] was theorized and put to the test by Gell-Mann and Pais, and would eventually lead to a ground breaking result in not only CP violation but the discovery of another generation of quarks. It was seen that the neutral Kaon, a meson of non-zero strangeness was decaying to pions of zero strangeness. This implied decay via the weak interaction which was believed to conserve CP. While the states \( |K^0\rangle \) and \( |\bar{K}^0\rangle \) are not eigenstates of CP, a linear combination of them create eigenstates of definite CP behavior

\[
K^0_S = \frac{1}{\sqrt{2}} (|K^0\rangle - |\bar{K}^0\rangle), \quad K^0_L = \frac{1}{\sqrt{2}} (|K^0\rangle + |\bar{K}^0\rangle),
\]

so that

\[
CP |K^0_S\rangle = + |K^0_S\rangle, \quad CP |K^0_L\rangle = - |K^0_L\rangle.
\]

To conserve CP and angular momentum, \( |K^0_S\rangle \) would decay to two pions while \( |K^0_L\rangle \) would decay to three pions. Note, it’s possible to construct a CP = +1 state of three pions with the right combination of J values; but this still does not change the fact that \( K_L \) cannot decay to two pions. The S and L in those states stand for short and long due to their relative lifetimes. The \( 2\pi \) decay rate is much shorter so in a beam experiment, most of the \( K_S \)’s should decay near the source of the beam and down the line should be a beam of pure \( K_L \)’s. The lifetimes are \( \tau_S = 0.895 \cdot 10^{-10} \) s and \( \tau_L = 5.22 \cdot 10^{-8} \) s so in most beam experiments, the \( K_S \)’s are gone after a few centimeters. Then, the way to test for CP violation is to see whether there are two pion decay products far down the beam line. The experiment by Cronin and Fitch in 1964 saw 45 two pion events out of 22,700 decays at the end of their 57 ft beam length. Thus, this was evidence that the \( K_L \) state was not a perfect eigenstate of CP. Meaning the long lived Kaon is a mixture of states that can decay to two or three pions. This was a huge discovery, much greater than the discovery of parity violation. With parity violation, it was observed that all neutrinos are left-handed so parity is maximally violated in weak interactions. This CP violation was much smaller and was first incorporated into the Standard Model by including a phase factor in the Cabibo-Kobayashi-Maskawa (CKM) matrix. This extra phase implied a third generation of quarks existed and was indeed correct.

Furthermore, in 1974 Gjesdal et al. showed that for the 41% of \( K_L \) that actually decay to just one pion, still with CP = -1, there was an actual preference for decay to matter vs antimatter. The decays are

\[
|K^0_L\rangle = \pi^+ + e^- + \bar{\nu}_e \quad \text{or} \quad |K^0_L\rangle = \pi^- + e^+ + \nu_e.
\]

If \( K_L \) were a pure eigenstate of CP, there would be an equal amount of the two decays. But Gjesdal showed that the long Kaon decays into the positron state more often than into the electron state. It was only by a fractional amount of \( 3.3 \cdot 10^{-3} \) which actually is on par with the CP violating strength in Cronin
and Fitch’s beam experiment of $2.24 \cdot 10^{-3}$. This distinct, unequal treatment of matter and antimatter from the violation of CP invariance suggested such a non-invariance is responsible for the dominance of matter over antimatter in the universe. Thus, shedding more light on CP violation, such as with the nEDM experiment, will help resolve the asymmetry between matter and antimatter.

Lastly, further evidence for weak interaction CP violation was theorized in 1981 by Carter and Sanda in regards to neutral B mesons. In 2001, a much larger CP violating strength compared to the neutral Kaons was found at SLAC and KEK for the decays:

$$B^0 \rightarrow K^+ + \pi^-,$$  \hspace{1cm} (1.21)

$$\bar{B}^0 \rightarrow K^- + \pi^+.$$  \hspace{1cm} (1.22)

The decay of equation 21 is 13% more common than its CP mirroring decay of Equation 22.

1.2.4 Time Reversal

Time reversal is much harder to test than P and/or C. There are no particles that are eigenstates of T - a particle cannot be shown to be identical to itself moving backward in time. In chemistry, the principle of detailed balance states that each elementary process should be brought to equilibrium by its reverse process; at equilibrium, the number of processes going from A to B should equal those going from B to A. In terms of the strong and electromagnetic interactions, the decay $n + p \rightarrow d + \gamma$ and its reverse $d + \gamma \rightarrow n + p$, should have the same reaction rate in either direction given the same momentum, energy, etc. Such processes have been checked for their reaction rates as a test of T invariance but its the weak interaction where CP symmetry fails that needs to be tested. However, reversing typical weak interaction decays are very hard in practice. This is usually due to either the strong and electromagnetic interaction taking dominance over the weak force’s strength or difficulty measuring neutrino properties. This has compelled researchers to search elsewhere: the electric dipole moment of an elementary particle. As previously mentioned, an EDM of an elementary particle that has no degeneracy would violate parity, as well as CP, but would also violate T since spin changes sign under T while the dipole moment would not. The evidence of CP violation also implies T violation.

1.3 History and Current Experimental Goals

For a neutron, an overall neutral particle that was once thought to be elementary, a neutron electric dipole moment (nEDM) would come about from the charge distribution of quarks making up the neutron. The search for an nEDM was only first proposed by E.M. Purcell and N.F. Ramsey in the 1950s because its existence would violate symmetries most physicists believed to be strictly conserved. As more symmetry violations were found in experiments I discussed in the last section, it became clear that theory beyond the Standard Model (SM) was needed to describe the observed symmetry violations and for a prediction of EDMs of elementary particles [Gol94]. Specifically, the SM predicts an nEDM to be $10^{-31}$e·cm and an electron EDM to be $10^{-40}$e·cm, the former being far outside current technologies.
reach. However, the theory of Supersymmetry predicts an nEDM to have an upper bound of $10^{-28}$e·cm which current experiments can get close to. Taken from [Fil09], the history of measuring an nEDM over time is shown in Figure 1.1.

![Figure 1.1](image)

**Figure 1.1** nEDM experimental upper limits over time and to which theory the limit belongs to. The current limits bring experiments to the Supersymmetry range.

As can be seen, the SM predictions are much lower and current technological capabilities puts experimental upper limits in the Supersymmetry regime. A more detailed history of measuring the nEDM I took from [Chu11] shows that the first nEDM measurement experiments used neutron scattering. Then experiments began using nuclear magnetic resonance (NMR) beam measurements. And now today, the use of ultracold neutrons (UCN) held in traps.
The experiment that I conduct research for is the nEDM at the Spallation Neutron Source (SNS) experiment. Its main competitors for an nEDM are ILL CryoEDM and PSI nEDM experiments. The former will use superfluid $^4$He similar to the SNS experiment; the latter will use solid deuterium as a source for UCN. ILL’s best measurements will aim for an nEDM limit of $2 \cdot 10^{-28} \text{e-cm}$. PSI’s will be $7 \cdot 10^{-28} \text{e-cm}$. Whereas SNS will be $1 \cdot 10^{-28} \text{e-cm}$. These values can be seen in Figure 1.3 from [Fil09].
The Fundamental Neutron Physics Beam Line at the SNS is used to fill the trap cells with cold neutrons. The multi-story apparatus is currently being built at Oak Ridge National Laboratory. Figure 1.4 shows the nEDM at SNS apparatus and demonstrates the large scale.

Before the experiment begins, a smaller scale testing apparatus will be used here at NCSU and TUNL. It will use neutrons from the PULSTAR reactor and is called 'Systematic and Operational Studies' (SOS). A side-by-side drawing of the SNS and SOS apparatuses is shown in Figure 1.5.
The $^4$He SNS and SOS will use is 1200 L and 5 L respectively. The cryogenic turnaround time at SNS is about 2-3 months making the study of systematic effects impractical. Whereas for the SOS, the cryogenic turnaround time is 2-3 weeks. What most these systematic effects are will be discussed next chapter.
2.1 Nuclear Magnetic Resonance

Nuclear magnetic resonance is a phenomenon that occurs when a static magnetic field is accompanied by a perpendicular, weak magnetic field oscillating at or near the Larmor frequency of the static field. It’s used in a multitude of different ways. In the nEDM experiment, it’s used to control the angles of spin in a very controlled fashion.

2.1.1 Classical and Quantum Description of Spin in a Static Field

2.1.1.1 The Classical Description

The equation of motion of a magnet, or a system containing a magnetic moment $\vec{\mu}$, in a magnetic field $\vec{B}$ is given by

$$\frac{d\vec{J}}{dt} = \vec{\mu} \times \vec{B}. \tag{2.1}$$

where $\vec{J}$ is the angular momentum. Then given the gyromagnetic ratio has been measured and $\vec{\mu} = \gamma \vec{J}$

$$\frac{d\vec{\mu}}{dt} = \vec{\mu} \times \gamma \vec{B}. \tag{2.2}$$

One can understand this equation better if I transform to the rotating frame as done in [Sli90]. To do this, consider the vector $\vec{\mu}(t)$ that can be written as $\vec{\mu} = i \mu_x + j \mu_y + k \mu_z$. I will take the time derivative of $\vec{\mu}$ and it will include a product rule because I will assume the unit vectors are not constant in time and
can rotate. They will rotate with velocity $\vec{\Omega}$ such that

$$\frac{d\hat{i}}{dt} = \vec{\Omega} \times \hat{i}. \quad (2.3)$$

Then $\vec{\mu}$ is

$$\frac{d\vec{\mu}}{dt} = i\frac{d\mu_x}{dt} + \mu_x \frac{d\hat{i}}{dt} + j\frac{d\mu_y}{dt} + \mu_y \frac{\hat{j}}{dt} + k\frac{d\mu_z}{dt} + \mu_z \frac{d\hat{k}}{dt}$$

$$= \frac{\partial \vec{\mu}}{\partial t} + \vec{\Omega} \times \vec{\mu} = \vec{\mu} \times (i\mu_x + j\mu_y + k\mu_z) \quad (2.4)$$

where the derivative using $\partial\partial$ is the derivative with respect to the lab frame. Setting equal Equation 2.2 and 2.4

$$\frac{d\vec{\mu}}{dt} = \frac{\partial \vec{\mu}}{\partial t} + \vec{\Omega} \times \vec{\mu} = \vec{\mu} \times (\gamma\vec{B} + \vec{\Omega}).$$

This transformation shows that the effective field has been transformed from $\vec{B}$ to $\vec{B} + \vec{\Omega}/\gamma$. Furthermore, if $\vec{B} = \hat{k} B_0$, I can transform to the frame rotating at $\Omega = -\gamma B_0 \hat{k}$ such that the effective field in this frame is zero. This is the basis on nuclear magnetic resonance and is powerful because the elimination of the static field enables more experimental control on $\vec{\mu}$.

2.1.1.2 The Quantum Description

For the quantum description, I will present the Hamiltonian, the eigenvalues and the way to construct eigenfunctions. Then I will derive the expectation values of the magnetic moments as done in [Sli90].

The Hamiltonian for a magnetic moment in a magnetic field is quite simple. Given $\vec{B} = \hat{k} B_0$

$$H = -\vec{\mu} \cdot \vec{B} = -\gamma \hbar B_0 S_z, \quad (2.6)$$

with eigenvalues $E = -m\gamma \hbar B_0$ for $m = -S, S + 1, ... S$. Allowed transitions for neighboring energy levels are

$$\Delta E = \hbar \omega = \gamma \hbar B_0 = \hbar \omega_0. \quad (2.7)$$

The time independent solutions to the Schrodinger equation $u_{S,m}$ can be used to construct the following time dependent solution

$$\Psi = \sum_{m=-S}^{+S} c_m u_{S,m} e^{-iE_m t/\hbar}, \quad (2.8)$$
where \( c_m \) are complex constants. The usual expression for the expectation value, for instance of the \( x \) component of the magnetic moment, is

\[
<\mu_x(t)> = \int \Psi^*(\tau)\mu_x\Psi(\tau)d\tau = \sum_{m,m'} \gamma \hbar c_m^* c_m <m'|S_x|m> e^{i(E_m-E_m)t/\hbar}
\]

(2.9)

\[
<m'|S_x|m> = \int u_{S,m}^* S_x u_{S,m} d\tau.
\]

To aid in the derivations, the spin raising and lowering operators are introduced

\[
S^+ = S_x + i S_y, \quad S^- = S_x - i S_y
\]

(2.10)

such that

\[
S_x = \frac{1}{2}(S^+ + S^-), \quad S_y = \frac{1}{2i}(S^+ - S^-).
\]

(2.11)

These operators have the following affect on the time independent solution:

\[
S^+ u_{S,m} = \sqrt{S(S+1) - m(m+1)} u_{S,m+1}
\]

\[
S^- u_{S,m} = \sqrt{S(S+1) - m(m-1)} u_{S,m-1}.
\]

(2.12)

For the spin 1/2 case, I will express the coefficients \( c_m \) generally as \( c_{1/2} = a e^{i\alpha} \) and \( c_{-1/2} = b e^{i\beta} \). Leaving out inner products that vanish, the expectation value for \( \mu_x \) is

\[
<\mu_x(t)> = \sum_{m,m'} \gamma \hbar c_m^* c_m <m'|S_x|m> e^{i(E_m-E_m)t/\hbar}
\]

\[
= \gamma \hbar \left[ c_{1/2} c_{-1/2} <1/2|S^+|1/2 > e^{-i\gamma B_0 t} + c_{-1/2} c_{1/2} <1/2|S^-|1/2 > e^{i\gamma B_0 t} \right]
\]

(2.13)

\[
= \gamma \hbar Re[ae^{i\alpha} be^{i\beta} e^{-i\omega_0 t}] = \gamma \hbar ab \cos(\omega_0 t + \alpha - \beta).
\]

For \( \mu_y \), I have

\[
<\mu_y(t)> = \sum_{m,m'} \gamma \hbar c_m^* c_m <m'|S_y|m> e^{i(E_m-E_m)t/\hbar}
\]

\[
= \frac{\gamma \hbar}{2i} \left[ c_{1/2} c_{-1/2} <1/2|S^+|1/2 > e^{-i\gamma B_0 t} - c_{-1/2} c_{1/2} <1/2|S^-|1/2 > e^{i\gamma B_0 t} \right]
\]

(2.14)

\[
= \gamma \hbar Im[ae^{-i\alpha} be^{i\beta} e^{-i\omega_0 t}] = -\gamma \hbar ab \sin(\omega_0 t + \alpha - \beta).
\]

Finally for \( \mu_z \)
<\mu_z(t)> = \sum_{m,m'} \gamma \hbar c^*_{m'} c_m \langle m' | S_z | m \rangle e^{i(E_{m'} - E_m)t/\hbar}

= \gamma \hbar [c^*_{1/2} c_{1/2} < 1/2|S_z|1/2 > e^0 + c^*_{-1/2} c_{-1/2} < -1/2|S_z|-1/2 > e^0]

= \gamma \hbar [\frac{1}{2} c^*_{1/2} c_{1/2} - \frac{1}{2} c^*_{-1/2} c_{-1/2}]

= \frac{1}{2} \gamma \hbar [ae^{-ia} be^{-ib} - be^{-ia} be^{-ib}] = \frac{1}{2} \gamma \hbar (a^2 - b^2). \tag{2.15}

What can be seen is <\mu_x(t)> and <\mu_y(t)> oscillate at the Larmor frequency while <\mu_z(t)> is independent of time. Hence, <\mu(t)>'s behavior is a vector making a fixed angle with the z-axis, precessing about the z-axis. This is exactly what we would expect given a static field along z and an initial position of \mu not parallel or anti-parallel to the z-axis.

2.1.2 Effect of a Weak Alternating Magnetic Field on Resonance

Suppose an alternating field \(B_x(t) = B_1 \cos \omega t\) is added to the setup with the static field \(\vec{B}_0 = B_0 \hat{k}\). This field can be decomposed into two counter rotating fields

\[
\vec{B}_R = \frac{B_1}{2} (\hat{i} \cos \omega t + \hat{j} \sin \omega t) \\
\vec{B}_L = \frac{B_1}{2} (\hat{i} \cos \omega t - \hat{j} \sin \omega t).
\tag{2.16}

As done in Slichter [Sli90], I can assume only \(\vec{B}_R\) exists because given the field is on resonance, \(\vec{B}_L\) can be neglected. For the sake of generality given resonance can occur in either direction, I will write \(\vec{B}_r = \vec{B}_1\) going forward. The equation of motion in the lab frame is

\[
\frac{d\vec{\mu}}{dt} = \vec{\mu} \times \gamma [\vec{B}_0 + \vec{B}_1(t)]. \tag{2.17}
\]

Given Equation 2.5, transforming to the frame rotating at \(\omega = \omega_0\) gives

\[
\frac{\delta \vec{\mu}}{\delta t} = \vec{\mu} \times \gamma \left(\vec{B}_0 + \frac{\omega_0}{\gamma} \hat{k} + B_1 \hat{i}\right) = \vec{\mu} \times \gamma B_1 \hat{i}. \tag{2.18}
\]

Dependence on the static field has vanished as well as the time dependence of the oscillating field. Furthermore, whether away from resonance or on it, the magnetic moment precesses about the effective field \((B_1, 0, B_0 - \omega/\gamma)\). It is through this mechanism that orientations of spins are controlled. For instance in the nEDM experiment, the UCN and \(^3\)He will be highly polarized in the same z direction and then 'moved' into the x-y plane. The manner in which they are moved to the x-y plane is by applying a \(\pi/2\) pulse using a weak oscillating field on resonance. On resonance, the effective field is solely along x such that a pulse of \(B_1\) applied for a time \(t_p\) can rotate the spins an angle \(\pi/2 = \gamma B_1 t_p\). The duration of \(t_p\) for a \(\pi/2\) rotation depends on the strength of \(B_1\) as well as \(\alpha = \gamma_3/\gamma_n\).

To treat this oscillating field quantum mechanically so I can solve for expectation values, I'll start with the following total field and apply the time dependent Schrodinger equation
where \( \phi \) which is just the Schrödinger equation with the effective field and effective Hamiltonian as previously mentioned. After some algebraic manipulation, the transformed Schrödinger equation is

\[
\frac{\hbar}{i} \frac{\partial \Psi'}{\partial t} = -\hat{\mathbf{B}}(t)\Psi = -\gamma \hbar [B_0 S_z + B_1 (S_x \cos \omega t + S_y \sin \omega t)]\Psi. \tag{2.19}
\]

In a frame rotating at \( \omega_z \) about the z-axis, spin operators and \( \Psi \) transform as

\[
\begin{align*}
S_x' &= e^{-iS_z \phi} S_x e^{iS_z \phi} = S_x \cos \phi + S_y \sin \phi \\
S_y' &= e^{-iS_z \phi} S_y e^{iS_z \phi} = -S_x \sin \phi + S_y \cos \phi \\
S_z' &= e^{-iS_z \phi} S_z e^{iS_z \phi} = S_z
\end{align*}
\] \tag{2.20}

where \( \phi = \omega_z t \). From Equation 2.19 and using Equation 2.20, the Hamiltonian can be written as

\[
H = -\gamma \hbar (B_0 S_z + B_1 e^{-i\omega_z t S_z} e^{i\omega_z t S_z}). \tag{2.21}
\]

After some algebraic manipulation, the transformed Schrödinger equation is

\[
\frac{\hbar}{i} \frac{\partial \Psi'}{\partial t} = -[\hbar (\omega_z + \gamma B_0) S_z + \gamma \hbar B_1 S_x] \Psi', \tag{2.22}
\]

which is just the Schrödinger equation with the effective field and effective Hamiltonian as previously mentioned. Furthermore, the relation of \( \Psi'(t) \) to \( \Psi'(0) \) is via a time evolution operator such that \( \Psi(t) = e^{-i\omega_z t S_z} e^{-iH't/\hbar} \Psi'(0) \). For the expectation values, I will assume \( B_1 \) is applied at resonance so that our reference frame is rotating at \( w_z = \gamma B_0 \), \( H = -\gamma \hbar B_1 S_x \). Initially magnetization \( M_0 \) is along \( \hat{k} \) such that \( < \mu_z(0) > = M_0 \) and the other components are zero. Defining \( \omega_1 = \gamma B_1 \), the expectation value for \( \mu_x \) is

\[
< \mu_x(t) > = \int \psi^*(t) \mu_x \psi(t) d\tau = \gamma \hbar \int e^{-i\omega_z t S_z} e^{-i\hbar H t} \psi(0)^*(S_x) e^{-i\omega_z t S_z} e^{-i\hbar H t} \psi(0) d\tau
\]

\[
= \gamma \hbar \int \psi(0)^* e^{i\hbar H t} e^{i\omega_z t S_z} S_x e^{-i\omega_z t S_z} e^{i\hbar H t} \psi(0) d\tau
\]

\[
= \gamma \hbar \int \psi^*(0) e^{-i\gamma B_1 S_z t} [S_x \cos \omega_z t + S_y \sin \omega_z t] e^{i\gamma B_1 S_z t} \psi(0) d\tau
\]

\[
= \gamma \hbar \int \psi^*(0) [S_x \cos \omega_z t + \sin \omega_z t (S_y + S_z \sin \omega_1 t) S_z \sin \omega_1 t] \psi(0) d\tau
\]

\[
= < \mu_x(0) \cos \omega_z t + < \mu_y(0) \sin \omega_z t \cos \omega_1 t > + < \mu_z(0) \sin \omega_z t \sin \omega_1 t >
\]

\[
= M_0 \sin \omega_z t \sin \omega_1 t.
\]
For \( \mu_y \) I have

\[
< \mu_y(t) > = \int \psi^\ast(t) \mu_y \psi(t) d\tau = \gamma \hbar \int \psi^\ast(0) e^{i(1/\hbar)Ht} e^{i\omega_z t S_z} S_y e^{-i\omega_z t S_z} e^{-i(1/\hbar)Ht} \psi(0) d\tau
\]

\[
= \gamma \hbar \int \psi^\ast(0) e^{-i\gamma B_1 t} [-S_x \sin \omega_z t + S_y \cos \omega_z t] e^{i\gamma B_1 t} \psi(0) d\tau
\]

\[
= \gamma \hbar \int \psi^\ast(0) [-S_x \sin \omega_z t + \cos \omega_z t (S_y \cos \omega_1 t + S_z \sin \omega_1 t)] \psi(0) d\tau
\]

\[
= - < \mu_x(0) > \sin \omega_z t + < \mu_y(0) > \cos \omega_z t \cos \omega_1 t + < \mu_z(0) > \cos \omega_z t \sin \omega_1 t
\]

\[
= M_0 \cos \omega_z t \sin \omega_1 t
\]

And finally, for \( \mu_z \)

\[
< \mu_z(t) > = \int \psi^\ast(t) \mu_z \psi(t) d\tau = \gamma \hbar \int [e^{-i\omega_z t S_z} e^{-(1/\hbar)Ht} \psi(0)]^\ast (S_z) (e^{i\omega_z t S_z} e^{-i(1/\hbar)Ht} \psi(0)) d\tau
\]

\[
= \gamma \hbar \int \psi^\ast(0) e^{i(1/\hbar)Ht} e^{i\omega_z t S_z} e^{-i\omega_z t S_z} e^{-(1/\hbar)Ht} \psi(0) d\tau
\]

\[
= \gamma \hbar \int \psi^\ast(0) e^{-i\gamma B_1 t S_z} e^{i\gamma B_1 t} \psi(0) d\tau = \gamma \hbar \int \psi^\ast(0) [-S_y \sin \omega_1 t + S_z \cos \omega_1 t] \psi(0) d\tau
\]

\[
= - < \mu_y(0) > \sin \omega_1 t + < \mu_z(0) > \cos \omega_1 t
\]

\[
= M_0 \cos \omega_1 t
\]

Thus, \( < \mu_z(t) > \) oscillates about the effective field \( B_1 \) in this rotating frame between values \( M_0 \) and \( -M_0 \) while the other components have a precession rate of the superposition of \( \omega_z + \omega_1 \) and \( \omega_z - \omega_1 \).

\section*{2.2 Bloch Equations}

\subsection*{2.2.1 Spin Bloch Equations in Lab and Rotating Frame}

\subsubsection*{Introduction to the Spin Bloch Equations}

From Equation 2.2, for a particle in a magnetic field, its magnetic moment will be subject to a torque that tends to align \( \vec{\mu} \) with \( \vec{B} \). Since the magnetic moment is always aligned along the spin vector, Equation 2.2 can be written as

\[
\frac{d\vec{S}(t)}{dt} = \vec{S} \times \gamma \vec{B}.
\]
These are the spin Bloch Equations I will use in my simulations. Furthermore, this idea can be extrapolated to the bulk property of magnetization $\vec{M}$ where $\vec{M}$ is essentially the sum over all $\vec{m}_i$’s across a volume. This allows for another form of Equation 2.2 as

$$\frac{d\vec{M}(t)}{dt} = \vec{M} \times \gamma \vec{B}. \tag{2.27}$$

For a static field along $+z$ and weak alternating field on resonance pointing along $x$, the magnetization is continuously changing its orientation with respect to the static field. There is a cycle of energy supplied by the alternating field and absorbed by it when the magnetization cycles through being parallel and antiparallel to the static field. In terms of an initial magnetization $M_0$ pointing along $+z$, $\vec{M}(0) = M_0 \hat{k}$, there is a continuous loss and recovery. When there is loss, the other components of magnetization can increase in magnitude. What this is called is relaxation. For this setup, $T_1$ (longitudinal) relaxation is when $M_z$ decreases due to depolarization while $T_2$ (transverse) relaxation is when $M_{x,y}$ experience loss due to dephasing, $T_1$ recovery or other loss mechanisms. Incorporating these into the Bloch Equations in Equation 2.27 gives

$$\frac{dM_x}{dt} = (\vec{M} \times \gamma \vec{B})_x - \frac{M_x}{T_2} \tag{2.28}$$

$$\frac{dM_y}{dt} = (\vec{M} \times \gamma \vec{B})_y - \frac{M_y}{T_2}$$

$$\frac{dM_z}{dt} = (\vec{M} \times \gamma \vec{B})_z - \frac{M_z - M_0}{T_1},$$

where the last part for the $M_z$ equation expresses how thermal equilibrium is when the magnetization points along $B_0$ and hence when $\vec{M} = M_0 \hat{k}$. For my simulations, I will not include relaxation terms because either they can be measured from the data or there will be no relaxation present.

### 2.2.1.2 Transforming to the Rotating Frame

I will briefly show how Equation 2.26 can be represented in a rotating frame. In my Comsol simulations, I mostly operated in the rotating frame. The Spin Bloch Equations in the lab frame are

$$\dot{S}_x = \gamma (B_z S_y - B_y S_z)$$

$$\dot{S}_y = \gamma (-B_z S_x + B_x S_z) \tag{2.29}$$

$$\dot{S}_z = \gamma (B_y S_x - B_x S_y).$$

In matrix form, $\vec{S} = \gamma B \vec{S}$, the matrix B is

$$\begin{pmatrix}
0 & B_z & -B_y \\
-B_z & 0 & B_x \\
B_y & -B_x & 0
\end{pmatrix} \tag{2.30}$$
where $\vec{S}$ and $\vec{S}_r$ are 3x1 column vectors. To transform to the rotating frame, I must transform the differential equations in a manner that accounts for the time derivative of the time dependent rotating matrix $R(t)$ that transforms $\vec{S}$ to the rotating frame $\vec{S}_r$.

$$\vec{S}(t) = R(t)\vec{S}_r(t). \quad (2.31)$$

The 3D rotation matrix for a rotation of $\omega_0 t$ about the z-axis is

$$R(t) = \begin{pmatrix} \cos \omega_0 t & -\sin \omega_0 t & 0 \\ \sin \omega_0 t & \cos \omega_0 t & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (2.32)$$

The spin vectors and rotation matrix are functions of time. I'll write Equation 2.29 as

$$\vec{S} = M\vec{S} = \begin{pmatrix} \dot{S}_x \\ \dot{S}_y \\ \dot{S}_z \end{pmatrix} = \gamma \begin{pmatrix} 0 & B_z & -B_y \\ -B_z & 0 & B_x \\ B_y & -B_x & 0 \end{pmatrix} \begin{pmatrix} S_x \\ S_y \\ S_z \end{pmatrix}, \quad (2.33)$$

where

$$M = \gamma \begin{pmatrix} 0 & B_z & -B_y \\ -B_z & 0 & B_x \\ B_y & -B_x & 0 \end{pmatrix}. \quad (2.34)$$

The time derivative applied to Equation 2.31 is

$$\frac{d}{dt} \vec{S} = \frac{dR}{dt} \vec{S}_r + R \frac{d\vec{S}_r}{dt} = M\vec{S} = M R \vec{S}_r$$

$$\rightarrow R\frac{d\vec{S}_r}{dt} = M R \vec{S}_r - \dot{R} \vec{S}_r, \quad (2.35)$$

$$\rightarrow \dot{\vec{S}}_r = [R^{-1} M R - R^{-1} \dot{R}] \vec{S}_r. \quad (2.36)$$

The terms in the brackets of Equation 2.36 are
\[
\begin{align*}
&\dot{\mathbf{R}} = \mathbf{R}^{-1} \mathbf{M} \mathbf{R} - \mathbf{R}^{-1} \dot{\mathbf{R}} \\
&= \begin{pmatrix} 
\cos \omega_0 t & \sin \omega_0 t & 0 \\
-\sin \omega_0 t & \cos \omega_0 t & 0 \\
0 & 0 & 1 
\end{pmatrix} \gamma \begin{pmatrix} 
0 & B_z & -B_y \\
-B_z & 0 & B_x \\
B_y & -B_x & 0 
\end{pmatrix} \begin{pmatrix} 
\cos \omega_0 t & -\sin \omega_0 t & 0 \\
\sin \omega_0 t & \cos \omega_0 t & 0 \\
0 & 0 & 1 
\end{pmatrix} \\
&\quad - \begin{pmatrix} 
\cos \omega_0 t & \sin \omega_0 t & 0 \\
-\sin \omega_0 t & \cos \omega_0 t & 0 \\
0 & 0 & 1 
\end{pmatrix} \omega_0 \begin{pmatrix} 
\cos \omega_0 t & -\sin \omega_0 t & 0 \\
\sin \omega_0 t & \cos \omega_0 t & 0 \\
0 & 0 & 0 
\end{pmatrix}
\end{align*}
\]

\[\gamma \begin{pmatrix} 
-B_z \sin \omega_0 t & B_z \cos \omega_0 t & B_z \sin \omega_0 t - B_y \cos \omega_0 t \\
-B_z \cos \omega_0 t & -B_z \sin \omega_0 t & B_z \cos \omega_0 t + B_y \sin \omega_0 t \\
B_y & -B_x & 0 
\end{pmatrix} \begin{pmatrix} 
\cos \omega_0 t & -\sin \omega_0 t & 0 \\
\sin \omega_0 t & \cos \omega_0 t & 0 \\
0 & 0 & 1 
\end{pmatrix} (2.37)
\]

\[
= \gamma \begin{pmatrix} 
0 & B_z & B_z \sin \omega_0 t - B_y \cos \omega_0 t \\
-B_z & 0 & B_x \cos \omega_0 t + B_y \sin \omega_0 t \\
-B_x \sin \omega_0 t + B_y \cos \omega_0 t & -B_x \cos \omega_0 t - B_y \sin \omega_0 t & 0 
\end{pmatrix} \begin{pmatrix} 
0 & -\omega_0 & 0 \\
\omega_0 & 0 & 0 \\
0 & 0 & 0 
\end{pmatrix}
\]

The only magnetic field along the +z is \( B_0 \), \( \gamma B_z = -\omega_0 \). Writing \( \gamma B_{x,y} = -\omega_{x,y} \) gives

\[\tilde{\mathbf{S}_r} = [\mathbf{R}^{-1} \mathbf{M} \mathbf{R} - \mathbf{R}^{-1} \dot{\mathbf{R}}] \mathbf{S}_r \]

\[= \begin{pmatrix} 
0 & 0 & -\omega_x \sin \omega_0 t + \omega_y \cos \omega_0 t \\
0 & 0 & -\omega_x \cos \omega_0 t - \omega_y \sin \omega_0 t \\
\omega_x \sin \omega_0 t - \omega_y \cos \omega_0 t & \omega_x \cos \omega_0 t + \omega_y \sin \omega_0 t & 0 
\end{pmatrix} \begin{pmatrix} 
\mathbf{S}_x \\
\mathbf{S}_y \\
\mathbf{S}_z 
\end{pmatrix}_r
\]

As a system of equations and dropping the r subscript for 'rotating', the Bloch Equations in the frame rotating at \( \omega_0 \) are
\[
\vec{S}_x = (-\omega_x \sin \omega_0 t + \omega_y \cos \omega_0 t)S_z \\
\vec{S}_y = (-\omega_x \cos \omega_0 t - \omega_y \sin \omega_0 t)S_z \\
\vec{S}_z = (\omega_x \sin \omega_0 t - \omega_y \cos \omega_0 t)S_x + (\omega_x \cos \omega_0 t + \omega_y \sin \omega_0 t)S_y.
\] (2.39)

2.3 Experimental Modes

2.3.1 nEDM at SNS Setup

The nEDM at SNS experiment will have cells of size 40cm × 7.5cm × 10cm. These cells will be filled with pure superfluid $^4$He cooled to about 0.4 K. Also in the cell will be polarized $^3$He with $x_3 \approx 10^{-10}$ and UCN who’s number density is about a factor of one billion smaller than the $^3$He. The two cells will be side-by-side with a high voltage electrode at the center and two ground electrodes on opposite sides. Hence, the static magnetic field and electric field will be parallel to the ground. This helps offset certain systematic effects such as the difference in height between the UCN and its comagnetometer $^3$He. Such a setup also points to the fact that the electric in one cell will point anti-parallel to the one in the other cell. The reason we want this in the experiment is to offset any systematic effects that are independent of $E$ or an even power of $E$. More will be talked about this later. Two important features of the superfluid $^4$He is that it will be used to bring cold neutrons down to ultracold temperatures and it has a high dielectric breakdown strength. So the electric field being used in the SNS experiments is much larger than any other previous nEDM experiment’s electric field. A higher $E$, longer measurement time $T_m$ (UCN stay in a trap much longer relative to higher temperature particles) and larger number of UCN $N$ all increase experiment sensitivity given the noise statistical sensitivity goes as

\[
\sigma(d_n) = \frac{\hbar}{2\alpha E T_m \sqrt{N}},
\] (2.40)

where $\alpha$ is a measure of polarization and will go from about 0.60 previously to 0.80 for this experiment. $T_m$ will be about 180s and the electric field will be about 75 kV/cm.

Regarding the neutrons, first a tail end of a Maxwell-Boltzmann distributed collection of neutrons are guided to the cell. These cold neutrons are polarized using a super-mirror and are filtered on their way into the cell such that only neutrons with wavelength about 8.9 Angstroms make it. This wavelength was chosen because its the energy of the neutrons that intersect with the $^4$He phonon dispersion curve shown in Figure 2.1. And therefore, the cold neutrons can down-scatter to UCN energy levels via collisions with $^4$He excitations (mostly phonons).
Figure 2.1 The neutron and $^4$He phonon dispersion curves showing where they intersect and what energy cold neutrons and down-scatter to UCN.

There are a number of loss mechanisms consistently taking neutrons out of the system but which can be mitigated. For instance, losses via wall absorption is mitigated with deuterated walls (deuterated polystyrene wall coating). The other significant UCN losses will come from beta decay, up-scattering and $^3$He absorption. Hence, the density of UCN in the cell will depend on a time constant of the form

$$\frac{1}{\tau_{\text{fill}}} = \frac{1}{\tau_\beta} + \frac{1}{\tau_{\text{up}}} + \frac{1}{\tau_w} + \frac{1}{\tau_3},$$

(2.41)

where the time constants on the right hand side are for beta decay (880s), up-scattering (70000s), wall absorption (>2000s) and $^3$He absorption (>10000s) respectively. Given the production rate of the Fundamental Neutron Beam Line (FNPB) filling the cells and time scales for losing UCN, the UCN density in a cell will be 170 UCN/cm$^3$ giving about $10^6$ UCN in the cells.

Essentially, the scheme of the experiment is to move the UCN and $^3$He spins to the transverse plane relative to the static field via a $\pi/2$ pulse on resonance and record the time dependence of UCN-$^3$He capture via scintillation signals from the products of that interaction

$$n + ^3He \rightarrow p + ^3H + 764\text{keV}.$$  

(2.42)

The absorption rate depends on the fields being applied such as the Larmor precession, systematic effects and the nEDM. However, the dependence on relative Larmor frequencies can drop out by critically dressing the spins. The spins start parallel when the absorption cross section is very close to 0. Whereas when the spins are antiparallel, the absorption cross section is on the order of 800kb. Clearly there is a spin dependent scattering length. When a capture occurs, the scintillation light from ionization in the superfluid helium will be at about 80nm. Based off the expectation value of $\vec{\sigma}_n \cdot \vec{\sigma}_3$, the scintillation signal in [Leu19] is given by
\[ \Phi(t) = N(t) \left[ \frac{\epsilon_\beta}{\tau_\beta} + \frac{\epsilon_3}{\tau_3} \left( 1 - P_3(t) P_n(t) \cos \theta_{3n}(t) \right) \right] + R_{BG}, \quad (2.43) \]

where \( N(t) \) is the number of UCN in a cell as a function of time, \( P_3(t) \) and \( P_n(t) \) are measures of polarization and begin very near 1, \( \theta_{3n}(t) = \theta_3(t) - \theta_n(t) \) is the average relative angle in the transverse plane between the \(^3\text{He}\) and UCN and \( \tau_3 \) is the time averaged UCN-\(^3\text{He}\) absorption time constant on the order of 40ns/\( x_3 \). \( R_{BG} \) accounts for background events and \( \epsilon_3 \approx 0.93, \epsilon_\beta \approx 0.33 \). What’s apparent is that the relative positions of the UCN and \(^3\text{He}\) spins in the transverse plane is of utmost importance. As I mentioned, there are several fields and effects at play affecting precession in the transverse plane. And for controlling these effects, there are two measurement modes.

### 2.3.2 Free Precession Measurement Mode

Free precession is the measurement mode that allows the UCN and \(^3\text{He}\) spins to freely precess in the transverse plane. The Hamiltonian in the presence of a magnetic field and electric field and non-zero dipole moment is

\[ H = -\vec{\mu} \cdot \vec{B} - \vec{d} \cdot \vec{E}, \quad (2.44) \]

so that a general difference in frequency between UCN and \(^3\text{He}\) after a \( \pi/2 \) pulse is

\[ \omega_{\text{free}} = \omega_3 - \omega_n = (\gamma_3 - \gamma_n) B_0 \pm \frac{2 e d_n E}{\hbar} + \delta \omega_3 - \delta \omega_n, \quad (2.45) \]

where the last two terms account for systematic effects. The phase angle UCN and \(^3\text{He}\) are building up, \( \theta_{3n} \), is such that neutron capture will occur at periodic times. Given only a static field and an nEDM term, the relative angle of the spins will be

\[ \theta_{3n}(t) = \left[ (\gamma_n - \gamma_3) B_0 \pm \frac{2 e d_n |E|}{\hbar} \right] t + \phi_0 \equiv \omega_{3n}^\pm t + \phi_0, \quad (2.46) \]

where \( \phi_0 \) is the relative phase at the start of measurement and is ideally near 0. The \( \pm \) refers to whether \( \vec{B}_0 \) and \( \vec{E} \) are parallel or anti-parallel. \( \omega_3 \) will be measured using superconducting quantum interference devices (SQUIDs) which minus some systematic effects, will be a good sampling of the fields the UCN are experiencing. Given \( \gamma_3/\gamma_n \approx 1.112 = \alpha \), the first term in Equation 2.46 gives a predictable contribution to the scintillation rate. After all, its the second term that is the unknown and is being measured. The scintillation rate ends up taking the form of an exponentially decaying cosine function. The exponential decay comes from \( T_2 \) relaxation for the polarization's as well as from UCN losses. For transverse relaxations in polarization given by \( P_i(t) = P_i^0 e^{-t/T_{2,i}} \) where \( T_{2,i} \) is on the order of 20000 s, the scintillation rate will be

\[ \Phi(t) = N(t) \left[ \frac{\epsilon_\beta}{\tau_\beta} + \frac{\epsilon_3}{\tau_3} \left( 1 - P_3^0 P_n^0 e^{-t/(T_{2,n} + T_{2,3})} \cos (\omega_{3n} t + \phi_0) \right) \right] + R_{BG}. \quad (2.47) \]
With the following approximation: $N(t) \approx N_0 e^{-t/\tau_{\text{rot}}}$. The results of Monte-Carlo simulations for Equation 2.47 in the free precession mode done by Kent Leung and shown in his paper [Leu19] are shown in Figure 2.2.

![Figure 2.2](image)

**Figure 2.2** The scintillation rate over time in blue on the bottom and a zoomed-in view during the first second on the top. In red is a best fit curve.

Finally, at the end of a measurement cycle, the $^3$He is no longer sufficiently polarized so it’s removed from the cell and new polarized $^3$He replaces it. For 300 days of running the free precession mode with $T_m \approx 1000$s and other parameters minimizing uncertainty, the $1\sigma$ precision gives an achievable bound for the nEDM to be: $\sigma_{d_n} \approx 3 \cdot 10^{-28}$ e·cm.

### 2.3.3 Dressed $^3$He-UCN Measurement Mode

Spin dressing is discussed in later chapters and was a very important feature of my research. Spin dressing is when a spin vector that is undergoing Larmor precession in say the x-y plane, is forced
to nutate out of the plane due to a strong, off-resonance oscillating magnetic field. In this context, UCN and $^3$He will be dressed in such a way that their Larmor frequencies can be matched. These are effective Larmor frequencies since the undressed Larmor frequency gets diluted: $\omega_0 \rightarrow \omega_0 J_0(\omega_1/\omega)$ where $J_0(\omega_1/\omega) \equiv J_0(x)$ is the zeroth order Bessel function of the first kind. For example if the static field $B_0$ is along $+z$ and the dressing field $B_x = B_1 \cos \omega t$ oscillates between $\pm x$, with $\omega_1 = \gamma_1 B_1$ and $B_1 >> B_0$, the spins will oscillate back and forth out of the x-y plane while simultaneously precessing about the z-axis. Given UCN and $^3$He naturally have different gyromagnetic ratios such that their $\omega_0$'s are different, $B_x$'s affect on them is also different. They therefore move out of the x-y plane by different amounts thereby making the distance they travel different so that finally, they return to their starting points at the same time.

The Larmor frequency is effectively shifted by a factor of $J_0(x)$. However, as it will become abundantly clear later, this is only valid in the limit $\omega_0 << \omega$. But given this assumption, there's a clear condition for the UCN and $^3$He to have equal effective Larmor frequencies $\omega_n$ and $\omega_3$

$$\omega_n - \omega_3 = 0 = -\gamma_n B_0 J_0\left(\frac{\gamma_n B_1}{\omega}\right) + \gamma_3 B_0 J_0\left(\frac{\gamma_3 B_1}{\omega}\right)
$$
$$= -\gamma_n B_0 J_0\left(\frac{\gamma_n B_1}{\omega}\right) + a \gamma_n B_0 J_0\left(\frac{a \gamma_n B_1}{\omega}\right) = \omega_0 \left[ J_0\left(\frac{\omega_1}{\omega}\right) - a J_0\left(\frac{a \omega_1}{\omega}\right) \right] = \omega_0 \left[ J_0(x) - a J_0(ax) \right].$$

Going forward, $\omega_1$ will be defined using $\gamma_n$ unless otherwise stated: $\omega_1 = \gamma_n B_1$. A solution to the condition only relies on what's in the brackets of Equation 2.48 and there are infinite values of x for the solution. A plot showing four possible solutions to the condition is shown in Figure 2.3.
Figure 2.3 The Bessel function terms in the brackets of Equation 2.48 make up the critical dressing condition. A zero crossing is a solution.

The zeroth order Bessel function of the first kind will be talked about more in later chapters but for now I will say that we want the lowest value of a solution shown in Figure 2.3 because this will give us the largest amplitude of \( J_0(x) \). And this matters specifically because the nEDM is diluted in the same fashion that \( \omega_0 \) is

\[
\frac{d_n E}{\hbar} \to \frac{J_0(x_c)d_n E}{\hbar},
\] (2.49)

where \( x_c \) is the critical dressing parameter and defined to be a solution to the critical dressing condition. The first solution in Figure 2.3 is \( x_c = 1.189018 \). Critically dressing the spins will remove the scintillation signal's dependence on the static field. For the magnitude of the dressing field \( B_1 \), \( x \) and \( \omega \) are the inputs since \( x = \gamma B_1 / \omega \) and we choose \( x = x_c \) and \( \omega / 2\pi \approx 2.5kHz \) (for the experiment).

Additionally, the dressing field has other benefits such as modulating it to offset a pseudomagnetic field. A pseudomagnetic field comes about due to the spin dependent scattering length for the UCN-\(^3\)He interaction. The field is only seen by the neutrons and therefore creates an unwanted asymmetry for the total fields the two species live in. With spin dressing, proper modulation about critical dressing can put the UCN forward and backward relative to the \(^3\)He such that symmetry about \( \theta_{3n} = 0 \) cancels the pseudomagnetic field affect. This will be discussed further in chapter 5. For 300 live days of the experiment, the 1\( \sigma \) precision for the dressed mode with modulation is \( \sigma_{d_n} = 1.6 \cdot 10^{-28} \) - a big step compared to the free precession mode at these sensitivities.
2.3.4 Systematic Effects

The pseudomagnetic field is one systematic effect briefly mentioned in the last section. But there are more effects I will briefly cover: magnetic field gradients, different spatial distributions, differences in trajectory motion and shifts induced solely from the motional field. Two very important systematic effects that require more attention and detail are geometric phases and pseudomagnetic field effects. The former will be explained next section and the latter will be explained in a later chapter.

Magnetic field gradients will inevitably exist even with great effort put into maintaining a constant $B_0$ field. Certain parts of the apparatus will mitigate gradients such as earth canceling magnetic field coils and a double layer magnetically shielded enclosure. But given even a small gradient in the $z$ direction, $G_z = \frac{\partial B_0}{\partial z}$, Maxwell’s Equations stating that the divergence of a magnetic field is zero means gradients in the $x$ or $y$ or both directions will exist. For ease of calculations and which are near realistic to first order, the gradients I will use throughout this paper will have cylindrical symmetry. This can be written as

\[ G_x + G_y + G_z = 0, \quad G_x = G_y \]
\[ \rightarrow G_x = -\frac{1}{2} \frac{\partial B_0}{\partial z}, \quad G_y = -\frac{1}{2} \frac{\partial B_0}{\partial z}. \]  

(2.50)

Furthermore, linear gradient magnetic fields $b_x, b_y$ and $b_z$ will be $b_x = xG_x$ and so on. Gradients in all directions will influence frequency shifts so using a comagnetometer will help resolve what the UCN are experiencing.

The UCN and $^3$He have different energies and masses such that their average heights will differ by about 2mm. The UCN will have energies about equal or less than the Fermi potential of the walls, since higher energy UCNs will be lost. Given their very low energy, the gravitational potential energy will keep UCN lower than the Helium on average. This difference in height can have large effects given spatially dependent gradients (and therefore spatially dependent geometric phases) and $^3$He acting as a comagnetometer. As previously mentioned, the electrodes will be arranged in such a way so that electric field will be perpendicular to gravity. Of course the static field will be aligned perpendicular to gravity as well. It’s also worth noting that in a vacuum, the mass of $^3$He increases by a factor of 2.4. Given the much higher concentration of superfluid $^4$He to $^3$He and absence of viscosity, $^3$He will indeed have this larger mass.

The UCN and $^3$He have different dynamical trajectories. The UCN undergo essentially ballistic motion since their mean free paths in $^4$He is about 10km. However, there is a small amount of up-scattering that will take place via the same interaction that caused down-scattering. $^3$He on the other hand will scatter off phonons (with $n_3 : n_4 < 10^{-7}$ and $^4$He brought below 500mK, phonon collisions dominate) and therefore are diffusing in the cells. As referenced in [CS16], the a temperature dependent diffusion coefficient was measured to be

\[ D = \frac{1.6}{T^7}. \]  

(2.51)

The diffusion coefficient is related to collision time through the equation $D = \tau_c \frac{kT}{m}$ so that the collision...
An electric and magnetic field written as

$$E = \frac{\partial A}{\partial t}$$

And in the same fashion,

$$\partial \phi$$

gives the following electric field components

$$E_x = -\frac{\partial \phi}{\partial x} - \frac{\partial A_x}{\partial t} = \frac{1}{4\pi \epsilon} \frac{q}{\sqrt{1 - v^2}} \frac{x - vt}{y^2 + z^2}$$

$$E_y = -\frac{\partial \phi}{\partial y} - \frac{\partial A_y}{\partial t} = \frac{1}{4\pi \epsilon} \frac{q}{\sqrt{1 - v^2}} \frac{y}{y^2 + z^2}$$

$$E_z = -\frac{\partial \phi}{\partial z} - \frac{\partial A_z}{\partial t} = \frac{1}{4\pi \epsilon} \frac{q}{\sqrt{1 - v^2}} \frac{z}{y^2 + z^2}$$

For the magnetic field

$$B = \nabla \times A = \det \left( \begin{array}{ccc} \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ A_x & A_y & A_z \end{array} \right)$$

so that

$$B_x = 0, B_y = \frac{\partial A_z}{\partial x},$$

and

$$B_z = -\frac{\partial A_y}{\partial z}.$$  

Then given

$$A_x = v \phi,$$

I have:

$$\frac{\partial A_y}{\partial y} = v \frac{\partial \phi}{\partial y} = -v E_y,$$

$$B_z = v E_z.$$  

And in the same fashion,

$$\frac{\partial A_z}{\partial z} = -v E_z = B_y,$$

the result is that

$$\vec{B} = \vec{v} \times \vec{E}.$$  

There will not be a frequency shift solely dependent on the motional field because in the trap, $v \approx 0$. However, $v^2 \neq 0$ but the measurements between parallel and anti-parallel electric fields will cancel out the squared motional field’s affect. A geometric phase is linear in $B_m$ and since $B_m$ couples to magnetic field gradients, the

$$\tau_c = 1.6 \frac{m}{kT^8}. \quad (2.52)$$

The motional field, $B_m = \frac{\vec{B} \times \vec{E}}{c}$ (in cgs units), arises when a charged particle moves through an electric field as seen from the particle’s frame of reference. One way it can be shown to exist is by applying a Lorentz transformation to a 4-potential $A_\mu = (\phi, \vec{A})$ for a particle moving in the $x$ direction with velocity $v_x = v$ and charge $q$. Applying the Lorentz transformation (with $c = 1$), the potentials become

$$\phi = \frac{1}{4\pi \epsilon} \frac{q}{\sqrt{1 - v^2}} \left[ \frac{(x - vt)^2}{1 - v^2} + y^2 + z^2 \right]^{1/2},$$

$$A_x = \frac{1}{4\pi \epsilon} \frac{q}{\sqrt{1 - v^2}} \left[ \frac{(x - vt)^2}{1 - v^2} + y^2 + z^2 \right]^{1/2},$$

$$A_y = A_z = 0. \quad (2.53)$$

A geometric phase is linear in $B_m$ and since $B_m$ couples to magnetic field gradients, the
effect will not be offset by an ensemble average or electric field direction flipping.

2.4 Geometric Phases

Geometric phases are possibly the most important systematic effect to understand. The reason is because the frequency shift they cause will be linearly proportional to the electric field. So not only will they remain after measurements for $\vec{E}$ parallel and antiparallel to $\vec{B}_0$, but their signal is indistinguishable to the nEDM signal. The effect is very small but given the incredible precision of the experiment, accounting for the 'false edm signal' is very important.

2.4.1 Classical Approach

To start, the false edm signal comes from a phase a state acquires over the course of a complete cycle in a parameter space. For an adiabatic process that does not alter the eigenstate, the geometric phase can be written as

$$c_n(T) = c_n(0)e^{i\gamma_n T}, \quad (2.57)$$

where $T$ is the time of a complete cycle in the parameter space. An intuitive example of this is with a Foucault pendulum. There is actually not a necessity of adiabaticity for a geometric phase to exist. A Berry's phase for when the process is adiabatic is just a special case. For reference, the adiabatic limit is for $\omega_0 \tau_{corr} > 1$ where $\tau_{corr}$ is the time scale for the correlation functions that I will mention shortly to go to zero. For no or little gas collisions and large field inhomogeneities, $\tau_{corr}$ is on the order of the time between wall collisions which I will assume to be

$$\tau_w = \frac{2R}{v} \sin \alpha, \quad (2.58)$$

where $R$ is the radius of the cylindrical trap, $v$ is the velocity of the particles under question and $\alpha$ is the angle at which the particle underwent specular reflection off a wall. Then for $B_0 = 30$ mG, $R = 0.235$ m, $v_{uc,n} = 5$ m/s and $v_3 = 35$ m/s and choosing $\alpha = \pi/4$, $\omega_0 \tau_w = 36.54$ and $\omega_0 \tau_3 \tau_w = 5.80$.

In the nEDM experiment, the false edm signal will be created through cycles in the magnetic field parameter space and specifically, the coupling of the magnetic field gradients with the motional magnetic field. The coupling can be seen classically be observing how the fields transform in the rotating frame and then back to the lab frame. For $\vec{B}_0 = B_0 \hat{k}$, $\vec{E} = -E \hat{k}$, $\vec{G}_z = \frac{\partial B_0}{\partial z} \hat{k}$, $\vec{B}_r = \frac{\partial B_0}{\partial z} \hat{r}$ and $\vec{B}_m = \vec{E} \times \frac{\gamma}{\tau} \hat{z}$ and in the frame rotating at $\omega_{r=R}$, the magetnic fields are

$$B(R) = B(R)_r \pm B(R)_m = aR - \frac{\omega R E}{c}$$

$$B^2 = \left(B_0 - \frac{\omega R}{\gamma}\right)^2 + B_R^2, \quad B' \equiv \left(B_0 - \frac{\omega R}{\gamma}\right) \quad \text{assume } B_R << B_0$$

$$B = B' \left(1 + \frac{B_R^2}{B^2}\right) \approx B' \left(1 + \frac{B_R^2}{2B'^2}\right) = B' + \frac{B_R^2}{2B'}.$$
Transforming back to the lab frame by adding an \(\frac{\omega E}{\gamma}\) gives

\[
B_{t,ab} = B_0 + \frac{B_R^2}{2(B_0 - \omega_R / \gamma)} = B_0 + \frac{(aR - \omega_RE/c)^2}{2(B_0 - \omega_R / \gamma)},
\]

(2.60)

so that the term linear in E term is

\[
\delta B_{RE} = -\frac{aR^2\omega RE}{c(B_0 - \omega_R / \gamma)} \to \frac{\gamma^2aE^2}{c(\omega_0^2 - \omega_R^2)},
\]

(2.61)

\[
\approx -\frac{aR^2\omega_R^2E}{cB_0^2} \frac{\omega_R}{\gamma} \ll B_0 \quad \text{or} \quad \approx \frac{\gamma^2aR^2E}{c} \frac{\omega_R}{\gamma} \gg B_0.
\]

The step that took the expression from a field to a frequency also averaged over rotation direction. What’s been shown is there is a frequency shift that is linearly proportional to the electric field.

### 2.4.2 Quantum Mechanical Approach

For a more complete derivation, I will use the quantum mechanical density matrix as done in [Gol94]. For a spin 1/2 particle the Hamiltonian can be written as

\[
H = H_0 + H_1(t) = -\frac{\omega_0}{2}\sigma_z - \frac{\omega_x(t)}{2}\sigma_x - \frac{\omega_y(t)}{2}\sigma_y = H_0 - (b^*\sigma_+ + b\sigma_-),
\]

(2.62)

where \(\sigma_{\pm} = \frac{1}{2}(\sigma_x \pm \sigma_y)\), \(b = \frac{1}{2}(\omega_x + i\omega_y)\), \(\omega_x = ax + \frac{\gamma E}{c}v_y\) and \(\omega_y = ay i\frac{\gamma E}{c}v_x\). On the Bloch sphere, a generalized density matrix in terms of spherical Pauli matrices and its time evolution is

\[
\rho = 1 + \rho_{10}\sigma_z + \rho_{11}\sigma_+ + \rho_{1-1}\sigma_- = \begin{pmatrix} 1 + \rho_{10} & \rho_{11} \\ \rho_{1-1} & 1 - \rho_{10} \end{pmatrix},
\]

(2.63)

\[
\frac{d\rho}{dt} = -i[H_0 + H_1(t), \rho],
\]

with \(\hbar = 1\). To remove the density matrix’s dependence on \(H_0\), I will transform to the frame rotating at \(\omega_0\). This will also transform \(H_1\) in the following manner

\[
H_1(t) \to \text{transforms} \to e^{iH_0t}H_1(t)e^{-iH_0t}.
\]

(2.64)

And using time dependent perturbation, an approximation of the density matrix up to second order can be written as

\[
\rho(t) = \rho(0) - \int_0^t [H_1(t'), \rho(0)] dt' - \int_0^t dt' \int_0^{t'} dt''[H_1(t'), [H_1(t''), \rho(0)]],
\]

\[
-\frac{d\rho}{dt} = -[H_1(t), \rho(0)] - \int_0^t d\tau [H_1(t), [H_1(t-\tau), \rho(0)]]
\]

(2.65)

\[
= -\int_0^t d\tau [H_1(t), [H_1(t-\tau), \rho(0)]] = \Gamma \rho(t),
\]

\]

29
where \( \tau = t - t' \) and \( \Gamma \) is defined as the relaxation matrix. \([H_i(t'), \rho(0)]\) vanished due to no correlation between \( \rho \) and the fluctuating Hamiltonian and from an ensemble average. If the perturbation is weak, \( \rho(0) \) can be replaced by \( \rho(t) \). The innermost commutator gives

\[
[H_i(t - \tau), \rho(t)] = e^{-i\omega_0 t} b^* \begin{pmatrix} -\rho_{11} - 2\rho_{10} & 0 \\ 0 & \rho_{11} - 2\rho_{10} \end{pmatrix} e^{i\omega_0 t} b' \begin{pmatrix} \rho_{11} & 0 \\ -2\rho_{10} & -\rho_{11} \end{pmatrix},
\]

where a \( b' \) refers to \( \omega \)'s that are a function of \( t' = t - \tau \). Then the next commutator gives

\[
[H_i(t), [H_i(t - \tau), \rho(t)]] = -e^{-i\omega_0 [2t - \tau]} b^* b'^i \begin{pmatrix} 0 & 2\rho_{11} \\ 0 & 0 \end{pmatrix} + e^{-i\omega_0 \tau} b^* b' \begin{pmatrix} 2\rho_{10} & 0 \\ 0 & -2\rho_{10} \end{pmatrix} + e^{i\omega_0 \tau} b b'^i \begin{pmatrix} 2\rho_{10} & 0 \\ 0 & -2\rho_{10} \end{pmatrix} - e^{i\omega_0 [2t - \tau]} b b' \begin{pmatrix} 0 & 0 \\ 0 & 2\rho_{11} \end{pmatrix}.
\]

Throwing out terms involving \( 2\omega_0 \) that average away, the results for the time derivatives are

\[
\dot{\rho}_{10} = -4 \int \text{Re} \{ e^{i\omega_0 t} b^* b'^i \rho_{10} \} d\tau,
\]

\[
\dot{\rho}_{11} = -2 \int e^{-i\omega_0 t} b^* b' \rho_{11} d\tau,
\]

\[
\dot{\rho}_{1-1} = -2 \int e^{i\omega_0 t} b b'^i \rho_{1-1} d\tau,
\]

\[
\frac{d\rho}{dt} = \begin{pmatrix} \dot{\rho}_{10} & \dot{\rho}_{11} \\ \dot{\rho}_{11} & -\rho_{10} \end{pmatrix} = \Gamma \begin{pmatrix} 1 + \rho_{10} & \rho_{11} \\ \rho_{1-1} & 1 - \rho_{10} \end{pmatrix}.
\]

The frequency shift is given by the imaginary of the off-diagonal elements of the \( \Gamma \) matrix

\[
\text{Im}[\Gamma_{12} - \Gamma_{21}] = 2 \text{Im} \left\{ \int_0^t \left( e^{-i\omega_0 \tau} b^* b' - e^{i\omega_0 \tau} b b'^i \right) d\tau \right\}.
\]

The terms in the integral with the exponentials and \( b \)'s expanded are

\[
e^{-i\omega_0 \tau} b^* b' - e^{i\omega_0 \tau} b b'^i = (\cos \omega_0 \tau - 2i \sin \omega_0 \tau) \frac{1}{2} (\omega_x(t) - i\omega_y(t)) \frac{1}{2} (\omega_x(t') + i\omega_y(t'))
\]

\[
- (\cos \omega_0 \tau + i \sin \omega_0 \tau) \frac{1}{2} (\omega_x(t) + i\omega_y(t))) \frac{1}{2} (\omega_x(t') - i\omega_y(t'))
\]

\[
= i[\cos \omega_0 \tau (\omega_x(t) \omega_y(t) - \omega_y(t) \omega_x(t')) - \sin \omega_0 \tau (\omega_x(t) \omega_y(t') + \omega_y(t) \omega_x(t'))].
\]

Finally, the frequency shift induced by an arbitrary weak field is

\[
\delta \omega = \int_0^t \left[ \cos \omega_0 \tau (\omega_x(t) \omega_y(t-t') - \omega_y(t) \omega_x(t-t')) - \sin \omega_0 \tau (\omega_x(t) \omega_y(t-t') + \omega_y(t) \omega_x(t-t')) \right].
\]
For the false edm shift we care about, I’ll expand the $\omega$’s and keep only terms linear in E. The other shifts that are proportional to $B^2$ (the gradient) and $E^2$ can be studied in ComSol as I will show, but they cancel out when the direction of E is reversed. For $a = \frac{\gamma E}{2} \frac{\partial R_0}{\partial x}$ and $b = \gamma E$, the linear in E shift is

$$
\delta \omega_{BE} = \int_0^t \cos \omega_0 \tau \left[ (a^2 x y' - a b x v_x' + b a v_y y' - b^2 v_y v_x' - a^2 y x' + a b y v_x' - b a v_x x' - b^2 v_x v_y') \right] d\tau
$$

$$
= -a b \int_0^t \cos \omega_0 \tau (x y' - y v_y' - v_x x') d\tau = -a b \int_0^t \cos \omega_0 \tau R(\tau) d\tau,
$$

(2.72)

where again, primed entities are functions of $t'$. Also, cross terms that will have no correlation, ie. $x y'$, were thrown out. $R(\tau)$ is defined as

$$
R(\tau) = \langle x(t) v_x(t - \tau) - v_y(t)(t - \tau) + y(t) v_y(t - \tau) - v_x(t) x(t - \tau) \rangle,
$$

(2.73)

which is the transverse position-velocity correlation functions. Thus, the conclusion here is that the false edm shift is proportional to the cosine Fourier transform of the transverse position-velocity correlation functions evaluate at $\omega_0$. The next step is to find appropriate expressions for the correlation functions so that a useful expression for the frequency shift can be obtained.

The cosine transform of the position-velocity correlation function can be written in terms of a position-gradient correlation function using integration by parts as done in [GP15]

$$
\int_0^\infty \cos \omega_0 \tau f(\tau) d\tau = \left[ \cos \omega_0 \tau \int_0^\tau f(\tau) d\tau \right]_0^\infty + \omega_0 \int_0^\infty \sin \omega_0 \tau \int_0^\tau f(\tau) d\tau d\tau.
$$

(2.74)

Expanding $a b$ and writing the sine transform as the imaginary component of a Fourier transform gives

$$
\delta \omega_{BE} = -\frac{\omega_0 \gamma^2 E}{c} \Im \left\{ \int_0^\infty e^{-i \omega_0 \tau} < B_x(t) x(t + \tau) + B_y(t) y(t + \tau) > d\tau \right\} - \frac{\gamma^2 E}{c} < B_x x + B_y y >
$$

(2.75)

Given linear gradients that take the form $b_x = x G_x$ and $b_y = y G_y$, Equation 2.75 can be written in terms of position autocorrelation functions. Moving to the Masoliver [Mas93] and Swank, Petukhov, Golub 2012 [CS12] papers, a position autocorrelation function may be written in terms of a conditional probability density $p(\vec{r}', t | \vec{r}_0, t_0)$ which is the probability of finding a particle at $\vec{r}'$ at time $t$ given it started at $\vec{r}_0$ at a time $t_0$. The position autocorrelation function is

$$
\langle x(t) x(t + \tau) \rangle = \int \int d^3 r d^3 r_0 x(\vec{r}) x(\vec{r}_0) p(\vec{r}, t | \vec{r}_0, t_0) p(\vec{r}', t_0),
$$

(2.76)

where $p(\vec{r}', t_0)$ is the probability of a finding a particle at $\vec{r}'$ at a time $t_0$ which for simplicity, can be made to be a constant distribution. So for a useful expression for the conditional probability density, the argument for continuous time random walks (CTRW) is used. The random walker (RW) or particle has
a probability of going from some point to another point undisturbed based off its initial angle, velocity and time of flight. Incorporate a probability density for the RW to be scattered off another particle and now the simple but full picture has been constructed. The probability of getting to \( \vec{r} \) at time \( t \) after being at \( \vec{r}' \) at time \( t_0 \), the conditional probability, is constructed using a conditional angular density, velocity filter, time of flight filter and a scattering probability density \( \rho(\vec{r}, t) \). For the conditional angular density \( \beta(\theta|\theta')d\theta \), the probability a single leg of the RW initially at \( \theta' \) will be followed by a turn made in the interval \( (\theta, \theta + d\theta) \) will have the first step uniformly distributed in \( (0, 2\pi) \) and all other turn angles are uniformly distributed in \( (-\pi, \pi) \) so that \( \beta(\theta|\theta') = \frac{1}{2\pi} \).

The scattering and particle conditional probability densities in two dimensions for a constant velocity are

\[
\rho(\vec{r}, t) = \frac{1}{2\pi} \left[ g(\vec{r}, t) + \int_0^t d^2\vec{r}' \int_0^t \rho(\vec{r}', \tau)g(\vec{r}' - \vec{r}, t - \tau)d\tau \right],
\]

\[
p(\vec{r}, t) = \frac{1}{2\pi} \left[ G(\vec{r}, t) + \int_0^t d^2\vec{r}' \int_0^t \rho(\vec{r}', \tau)G(\vec{r} - \vec{r}', t - \tau)d\tau \right],
\]

where \( g(\vec{r}, t) = f(\vec{r}, t)\psi(t) \) with \( f(\vec{r}, t) = \delta(x - vt\cos\theta)\delta(y - vt\sin\theta) \) and \( \psi = \frac{1}{\tau_c}e^{-t/\tau_c} \). And \( G(\vec{r}, t) = f(\vec{r}, t)\Psi(t) \) with \( \Psi = \int_0^\infty \psi(\tau)d\tau \).

\( f(\vec{r}, t) \) is the velocity filter and \( \psi \) and \( \Psi \) are the probability densities for the time spent \( t \) moving along a straight line before a turn via scattering and for times greater than \( t \) respectively. Taking the Fourier-Laplace transform (FLT) of \( \rho \) and \( p \), I can use the property that the FLT of a convolution is equal to the products of the individual FLT’s. \( \vec{r} \) will transform to \( \hat{q} \) and \( t \) will transform to \( s = i\omega \). Then the transformed quantities are

\[
\hat{\rho}(\hat{q}, s) = \frac{\hat{\rho}(q, s)}{2\pi - \hat{g}(q, s)}
\]

\[
\hat{p}(\hat{q}, s) = \frac{\hat{G}(q, s)}{2\pi - \hat{g}(q, s)}.
\]

Making use of the simple case of \( \psi(t) = \frac{1}{\tau_c}e^{-t/\tau_c} \) such that \( \hat{G}(q, s) = \hat{g}(q, s)\tau_c \), \( p \) becomes

\[
\hat{p}(q, s) = \frac{\hat{G}(q, s)}{2\pi - \frac{1}{\tau_c}\hat{G}(q, s)}.
\]

From here, the spectrum of the conditional probability can be found. But in reality, the velocities of the particles are not constant. In the nEDM experiment, the cold neutrons are taken from the low temperature part of a Maxwell-Boltzmann velocity distribution. So making the assumption that I can roughly use this distribution, the velocity distribution \( \alpha_N(\vec{v}) \) is introduced

\[
\alpha_N(\vec{v}) = \prod_{i=1}^N \left[ \frac{1}{2} \sqrt{\frac{2m}{\pi kT}} e^{-\frac{mv_i^2}{2kT}} \right].
\]

Equations 2.77 and 2.78 become
\[
\rho(\vec{r}, t, \vec{v}) = \frac{1}{2\pi} \left[ \alpha(\vec{v}) g(\vec{r}, t, \vec{v}) + \alpha(\vec{v}) \int d^2 \vec{r}' \int_0^t \rho(\vec{r}', \tau) g(\vec{r} - \vec{r}', t - \tau, \vec{v}) d\tau \right].
\]

(2.82)

\[
p(\vec{r}, t, \vec{v}) = \frac{1}{2\pi} \left[ \alpha(\vec{v}) G(\vec{r}, t, \vec{v}) + \alpha(\vec{v}) \int d^2 \vec{r}' \int_0^t \rho(\vec{r}', \tau) G(\vec{r} - \vec{r}', t - \tau, \vec{v}) d\tau \right].
\]

(2.83)

And analogous to \( \dot{\rho} \) in Equation 2.80

\[
\dot{\rho}(\vec{q}, s) = \int \alpha(\vec{v}) G(\vec{q}, s, \vec{v}) d^3 \vec{v} = \int \frac{\alpha(\vec{v}) G(\vec{q}, s, \vec{v}) d^3 \vec{v}}{1 - \int \alpha(\vec{v}) G(\vec{q}, s, \vec{v}) d^3 \vec{v}}
\]

(2.84)

where the \( \frac{1}{2\pi} \) normalization is instead being included in the transformation. I define \( F_N(\vec{q}, s) = \int \alpha(\vec{v}) G(\vec{q}, s, \vec{v}) d^N \vec{v} \) such that expanding \( F_N \) for \( N \) dimensions gives

\[
F_N(\vec{q}, s) = \int \alpha(\vec{v}) G(\vec{q}, s, \vec{v}) d^N \vec{v} = \int_0^\infty dt \int \alpha_N(\vec{v}) \sigma^{(N)}(\vec{x} - \vec{v} t) e^{-t/\tau_c - i \vec{q} \cdot \vec{x} - i t} dN \vec{x} d^N \vec{v}
\]

(2.85)

Integrating over the positions is trivial given the delta functions. Whereas integrating over the velocities and time involved completing the square in the exponential and making use of Gaussian integral properties. The velocity integral is from \(-\infty \) to \( \infty \) so that the result is a constant. However the time integral is from 0 to \( \infty \) which after \( \alpha \) substitution can be shown to give an error function. The result is

\[
F_N(\vec{q}, s) = \sqrt{\frac{2m}{\pi k T q^2}} e^{-z^2} \text{erfc}(z) \equiv F(q, z) \quad z(q, s) = \sqrt{\frac{m}{2k T}} \frac{1 + s \tau_c}{\tau_c q}.
\]

(2.86)

Putting this infrastructure to work using the method of images as done in [CS16] for a rectangle of size \((L_x, L_y, L_z)\), it was that shown that the spectrum of the \( x \) position autocorrelation function is \((s = i \omega)\)

\[
S_{xx}(\omega) = \sum_{n=0}^\infty \frac{4L_x^2}{\pi^4 q^4} p(|q_x| = \frac{\pi |n|}{L_x}, \omega).
\]

(2.87)

With cylindrical symmetry for the gradients and linear gradients, the linear in \( E \) frequency shift can be written as

\[
\delta \omega_{BE} = \omega \frac{\gamma^2 E G_z}{2c} \left[ 1 - m \left( S_{xx}(\omega) + S_{yy}(\omega) \right) + \frac{\gamma^2 E G_z}{2c} < x^2 + y^2 > \right].
\]

(2.88)

The linear in \( E \) shift is normalized by \( ab L^2 \) and the independent variable is \( \omega \tau_b \) where \( \tau_b = L \sqrt{\frac{m}{\pi k T}} \). In the experimental setup, there is dilute \(^3\)He Larmor precessing in superfluid \(^4\)He. The \(^3\)He collisions will be dominated by collisions with excitation's in the superfluid which will be phonons at these temperatures. The trap is a rectangle of dimensions \((L_x, L_y, L_z) = (10.2, 40, 7.6) \) cm. The \(^3\)He has an increased mass in the superfluid: \( m^*_{He} = 2.4 m_{He} \). The diffusion constant was experimentally measured to be
\[ D = \frac{1.6}{T}, \] \hspace{1cm} (2.89)

so that if \( v = \sqrt{\frac{kT}{m}} \) for \( D = v^2 \tau_c \)

\[ \tau_c = 1.6 \frac{m}{kT^8}. \] \hspace{1cm} (2.90)

To use \( \omega \tau_b \) as the independent variable, define \( \xi = \frac{\tau_c}{\tau_b} \), \( \omega' = \omega \tau_b \) and rearrange \( z \)

\[ z = \sqrt{\frac{m}{2kT}} \frac{1+s \tau_c}{\tau_c q} = \sqrt{\frac{m}{2kT}} \frac{(1+i \omega \tau_c) L \tau_c n \pi}{\tau_c n \pi} = \frac{1}{\sqrt{2} \tau_c} \frac{1+i \omega' \xi}{n \pi} = \frac{1}{\sqrt{2} n \pi} \frac{1+i \omega' \xi}{\xi}. \] \hspace{1cm} (2.91)

Writing the causal conditional probability as

\[ p(q, \omega) = \frac{\tau_c}{1-\frac{1}{\tau_c} F(q, \omega)} - 1 = \frac{\tau_c}{1-\sqrt{\frac{m}{2kT} \frac{1}{q \tau_c}} e^{zz} \text{erfc}(z)} - 1 \]
\[ = \frac{\tau_c}{1-\sqrt{\frac{m}{2kT} \frac{1}{n \tau_c}} e^{zz} \text{erfc}(z)} - 1 = \frac{\tau_c}{1-\sqrt{\frac{1}{2} \frac{1}{n \tau_c}} e^{zz} \text{erfc}(z)} - 1, \] \hspace{1cm} (2.92)

the spectrum of the position autocorrelation function is

\[ S_{xx}(\omega') = \sum_{odd} \frac{8 L_x^2}{\pi^4 n^4} \left[ \frac{\tau_c}{1-\sqrt{\frac{1}{2} \frac{1}{n \tau_c}} e^{zz} \text{erfc}(z)} - 1 \right]. \] \hspace{1cm} (2.93)

where actually \( z \) and \( \xi \) depend on whether \( L_x \) or \( L_y \) is being used for \( S_{xx} \) or \( S_{yy} \). \( S_{yy} \) is the same as \( S_{xx} \) except replace \( L_x \) with \( L_y \) and respective \( \tau_{bi} \) and \( \xi_i \). [CS16] used temperatures 300, 350, 400 and 450 mK and the results were

![Figure 2.4](image-url) Normalized linear in E frequency shift bounded to a length of 40 cm. Normalization was with \( ab L^2 \).
The experiment will take advantage of this fast drop off for the false edm signal. There is also a zero crossing near where the Helium will lie given the experiment’s parameters.
3.1 False EDM, $E^2$ and $B^2$ Frequency Shifts

3.1.1 Implementation in Comsol

Comsol can be used for a multitude of applications. I use it for tracking the individual trajectories of a particle in an ensemble. For instance, for specular wall collisions without gas collisions in a two dimensional circular trap, a particle will bounce off the walls with a constant angle $\alpha$. For obvious reasons, I want as many particles in my ensemble. Due to computation time and memory limits, I use 10,000 particles in a given simulation. I run a simulation for 2 seconds with time steps of 0.0001 seconds. Note, 2 seconds of simulation time is not computation time. My simulations are limited by not only simulation time but computer memory. Comsol creates thousands of temporary solution files when solving that fill up space fast. When running a new simulation, those temp files get automatically deleted so new ones can take their place. Therefore, I have to be careful with how many magnetic fields I include in a given parametric sweep. For 2D, Comsol will track the $x$, $y$, $v_x$ and $v_y$ of each particle at every time step.

For initial conditions, I make position density proportional to $\rho = 1$ meaning the particle position distribution will be homogeneous and isotropic. For the initial velocities

$$v_x = v_0 \cos \theta \quad v_y = v_0 \sin \theta$$

(3.1)
Where $\theta$ is uniformly distributed between 0 and $2\pi$. Then of course the following constraint will always hold

$$v_x^2 + v_y^2 = v_0^2$$  \hspace{1cm} (3.2)

And as usual on a Bloch sphere

$$S_x = \cos \theta \cos \phi$$
$$S_y = \cos \theta \sin \phi$$
$$S_z = \sin \theta$$  \hspace{1cm} (3.3)

With initial conditions

$$S_{x0} = 1 \hspace{0.5cm} S_{y0} = 0 \hspace{0.5cm} S_{z0} = 0$$  \hspace{1cm} (3.4)

For the number of particles, simulation and time step length, Comsol inputs 200 million sets of $x$, $y$, $v_x$ and $v_y$ into the differential equations for our auxiliary dependent variables $S_x$, $S_y$ and $S_z$

$$\frac{d\vec{S}}{dt} = \gamma (\vec{S} \times \vec{B}_{\text{eff}})$$  \hspace{1cm} (3.5)

$$\vec{B}_{\text{eff}} = (B_0 + Gz)\hat{k} - \frac{1}{2}G\hat{r} + \frac{E}{c^2}\hat{k} \times \vec{v}$$  \hspace{1cm} (3.6)

Frequencies can be extracted by either fitting the spin components or calculating $\frac{d\phi}{dt}$, which will be discussed in the next section.
3.1.2 Lab and Rotating Frame

The Larmor precession is described by \( \frac{d\phi}{dt} \) and then perturbations to this precession are described by \( \frac{d\theta}{dt} \). These perturbations look like nutations on the precession. They are induced by two systematic affects: inhomogeneities in the \( B_0 \) field and a motional field as seen from a particle’s perspective. In my research, I use the following fields

\[
\vec{B}_{0,xy} = \vec{B}_{0,r} = -\frac{\partial B_0}{\partial z} \frac{\vec{r}}{2}; \vec{B}_v = \frac{\vec{E} \times \vec{v}}{c}
\] (3.7)

At one point, I was exporting the data for \( S_x \) and \( S_y \) into Matlab and fitting the curves to find frequencies. That was tedious and time consuming. Edward Davis brought up the idea of calculating the frequency within ComSol using \( \frac{d\phi}{dt} \)

\[
\frac{d}{dt} \left( \frac{S_y}{S_x} \right) = \frac{\dot{S}_y S_x - \dot{S}_x S_y}{S_x^2} = \frac{\dot{S}_y S_x - \dot{S}_x S_y}{\cos^2 \theta \cos^2 \phi} = \frac{d\phi}{dt} \frac{1}{\cos^2 \phi} \rightarrow \frac{d\phi}{dt} = \frac{\dot{S}_y S_x - \dot{S}_x S_y}{S_x^2 + S_y^2}
\] (3.8)

Whether \( \frac{d\phi}{dt} \) is the Larmor frequency or a shift to it, depends on what frame I calculate it in. Originally, I was working in the non-rotating, dimensionful frame. In the non-rotating frame, \( \frac{d\phi}{dt} \) is the Larmor frequency, determined by \( B_0 \), plus or minus the frequency shift I’m looking trying to obtain. However in the rotating frame, \( \frac{d\phi}{dt} \) is the outright total frequency shift. And to extract a linear in \( E \) frequency shift I must find the difference between \( \frac{d\phi}{dt}(E+) \) and \( \frac{d\phi}{dt}(E-) \). Where as for the \( B^2 \) \( (E = 0) \) and \( E^2 \) \( (B = 0) \) shifts, \( \frac{d\phi}{dt} \) close to total contribution will be those shifts.

Something I thought was worth investigating was comparing the computation time of these four forms of Bloch equations: rotating frame dimensionless, rotating frame dimensionful, lab frame dimensionless and lab frame dimensionful. The effective fields and corresponding Bloch equations are shown in Table 3.1. Given which case you’re working in, \( \frac{d\phi}{dt} \) takes different explicit forms. For example, \( \frac{d\phi}{dt} \) in the rotating frame but with either dimensionless or dimensionful quantities both have \( \frac{d\phi}{dt} = \frac{-b_x S_x + b_y S_y S_z}{S_x^2 + S_y^2} \), but \( b_x \) and \( b_y \) have different expressions. Through doing simulations and \( \frac{d\phi}{dt} \) calculations, the computation time and evaluation took about the same time for all four cases. Thus, nothing was clearly advantageous in terms of time. However, as previously mentioned, \( \frac{d\phi}{dt} \) in the rotating frame is the outright shift. So computing in the rotating frame gets rid of the small step of subtracting the Larmor frequency from the \( B^2 \) and \( E^2 \frac{d\phi}{dt} \)’s. I also believe working with dimensionless units makes certain things more obvious such as the relative field strengths of the perturbation fields to \( B_0 \). Therefore, the data shown going forward will be from simulations in the rotating frame with dimensionless quantities.
Rotating, dimensionless:

\[
\begin{align*}
    b_x(\tau) &= -(\zeta u_x + \eta \dot{u}_y) \cos \tau - (\zeta u_y - \eta \dot{u}_x) \sin \tau \\
    b_y(\tau) &= -(\zeta u_y - \eta \dot{u}_x) \cos \tau + (\zeta u_x + \eta \dot{u}_y) \sin \tau
\end{align*}
\]

\[
\begin{bmatrix}
    \dot{S}_x^n \\
    \dot{S}_y^n \\
    \dot{S}_z^n
\end{bmatrix} = \begin{bmatrix}
    b_y S_z^n \\
    -b_x S_z^n \\
    -b_y S_x^n + b_x S_y^n
\end{bmatrix}
\]

Rotating, dimensionful:

\[
\begin{align*}
    B_x &= G q_x + v_y E / c^2, \quad B_y = G q_y - v_x E / c^2 \\
    b_x(t) &= \gamma(-B_x \cos \tau - B_y \sin \tau), \quad b_y(t) = \gamma(B_x \sin \tau - B_y \cos \tau)
\end{align*}
\]

\[
\begin{bmatrix}
    \dot{S}_x^n \\
    \dot{S}_y^n \\
    \dot{S}_z^n
\end{bmatrix} = \begin{bmatrix}
    b_y S_z^n \\
    -b_x S_z^n \\
    -b_y S_x^n + b_x S_y^n
\end{bmatrix}
\]

Lab, dimensionless:

\[
\begin{align*}
    b_x(\tau) &= -\zeta u_x - \eta \dot{u}_y, \quad b_y(\tau) = -\zeta u_y + \eta \dot{u}_x
\end{align*}
\]

\[
\begin{bmatrix}
    \dot{S}_x \\
    \dot{S}_y \\
    \dot{S}_z
\end{bmatrix} = \begin{bmatrix}
    -S_y + b_y S_z \\
    S_x - b_x S_z \\
    -b_y S_x + b_x S_y
\end{bmatrix}
\]

Lab, dimensionful:

\[
\begin{align*}
    B_x &= G q_x + v_y E / c^2, \quad B_y = G q_y - v_x E / c^2, \quad B_z = B_0 \\
    \dot{S}_x &= \gamma(S_y B_z - S_z B_y) \\
    \dot{S}_y &= \gamma(S_x B_z - S_z B_x) \\
    \dot{S}_z &= \gamma(S_x B_y - S_y B_x)
\end{align*}
\]

Where: \( \tau = \omega_0 t, \quad \vec{u} = \frac{T}{R}, \quad \vec{\dot{u}} = \frac{\vec{T}}{\kappa \omega_0}, \quad \zeta = \frac{RG}{2 \omega_0}, \quad \eta = \frac{R \omega_0 E}{c^2} \). In regards to how to get an output of \( \frac{d \phi}{dt} \) using
Comsol, I used a Global Evaluation from the Derived Values node as part of the Results node. In order to call variables like $b_x$ or $S_y$, a mathematical particle tracing operator needs to be used. Considering I need to average over my ensemble, I used

$$\frac{\text{pt.ptop1}\left(\frac{d\phi}{dt}\right)}{\text{pt.ptop1}(1)}$$

(3.9)

All pt.ptop1() does is it takes the sum of its argument across all particles at each given time step. So the denominator in Equation 3.9 is equal to 10,000 if I have 10,000 particles in my simulation. This expression alone produces a $\frac{d\phi}{dt}$ vs t graph that looks like a damped sinusoidal plot. The steady state behavior of $\frac{d\phi}{dt}$ is the average frequency or average frequency shift of the ensemble. Instead of extending my simulation to see where $\frac{d\phi}{dt}$ converges, I take a time average over the plot which is done using an operation selection in the global evaluation. I know this time average is a good proxy for the steady state behavior of $\frac{d\phi}{dt}$ because I took averages over intervals on $\frac{d\phi}{dt}$ and their average matched the total average.

### 3.2 Comparison to Theory

#### 3.2.1 Comsol Data vs. Barabanov Numerical Data

The paper [ALB06] outlines ways to calculate a linear in E frequency shift by finding analytical expressions for the correlation functions in different cases such as constant velocity, specular wall collisions with or without gas collisions. In my research, I’ve been using a fixed velocity with no gas collisions and specular wall collisions.

As previously shown, the linear in E shift can be written in terms of a position-velocity correlation function $R(\tau)$. And in the same fashion that I transform the position-velocity correlation function to a position-gradient correlation function, Barabanov uses the velocity correlation function $\psi(t)$

$$\psi(t) \equiv \langle \vec{v}_{x,y}(t) \cdot \vec{v}_{x,y}(0) \rangle$$

$$R(\tau) = 2 \int_0^{\tau} \psi(t) dt$$

(3.10)

Then given specular wall collisions and no gas collisions, Barabanov deduces the probability a trajectory bounces at an angle $\alpha$ by making use of its equivalence with the probability a trajectory’s closest approach to the center exists within a specified interval. For instance, a large $\alpha$ keeps a trajectory away from the center and vice versa. And for specular wall collisions, $\alpha$ is constant for a given particle. The probability a trajectory has an angle $\alpha$ is

$$P(\alpha) = \frac{4 \sin^2 \alpha}{\pi}$$

(3.11)

Where $R$ is the radius of the cylinder. And for this setup, $\psi(t)$ is actually a $\psi(\alpha, t)$
\[ \psi(\alpha, t) = \langle \vec{v}_{x,y}(t) \cdot \vec{v}_{x,y}(0) \rangle, \quad \psi(\alpha, 0) = v^2_{x,y} \] (3.12)

Barabanov then uses an averaging method whereby a total trajectory is made into a piece-wise function describing each chord between wall collisions. And because the velocity is constant, the velocity autocorrelation function is simply proportional to \( \cos \theta(t) \) from the dot product. The linear in \( E \) frequency shift is proportional to the cosine transform of \( \psi(\alpha, t) \) and then using this integral expression for a Bloch-Seigert shift

\[ -\Delta \omega(\alpha) = ab \int_{-\infty}^{\infty} \frac{\psi(\alpha, \omega)}{\omega^2 - \omega_0^2} d\omega \]

\[ = 2ab v^2 \sin^2 \alpha \sum_{m=-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\delta(\omega + \frac{2\alpha - 2\pi m}{\tau_w}) + \delta(\omega - \frac{2\alpha + 2\pi m}{\tau_w})}{\tau^2 \omega^2 (\omega^2 - \omega_0^2)} d\omega \] (3.13)

Then defining \( \delta_0 = \omega_0 R \sin \alpha / v = \omega' \sin \alpha \) and evaluating the integral, the result is

\[ -\Delta \omega(\alpha) = \left( \frac{v}{\omega_0} \right)^2 ab \left( 1 + \frac{\sin^2 \alpha \sin 2\delta_0}{2\delta_0 \sin(\delta_0 - \alpha) \sin(\delta_0 + \alpha)} \right) \] (3.14)

And integrating over all angles weighted by their probability

\[ \Delta \omega = \int_0^{\pi/2} P(\alpha) \Delta(\alpha) d\alpha = \int_0^{\pi/2} \frac{4 \sin^2 \alpha}{\pi} \left( \frac{v}{\omega_0} \right)^2 ab \left( 1 + \frac{\sin^2 \alpha \sin 2\delta_0}{2\delta_0 \sin(\delta_0 - \alpha) \sin(\delta_0 + \alpha)} \right) d\alpha \] (3.15)

Now, this expression can be used for comparison to my simulations. But instead, I saw that the shift that incorporated gas collisions actually was a much better comparison to my simulations, albeit, with the mean free path much larger than the trap size \( R \).

To include gas collisions, replace \( \delta_0 \) with \( \delta \) where

\[ \delta = \delta_0 \sqrt{1 + \frac{i}{\omega_0 \tau_c}} \] (3.16)

Where \( \tau_c \) is the average time between collisions. Using some algebra, \( \frac{i}{\omega_0 \tau_c} \) can be replaced by \( \frac{ir_0}{\omega} \) where \( r_0 = R/\lambda \), is the damping parameter and \( \omega' = \omega_0 R / \omega \). The numerical integration for no gas collisions and with gas collisions for varying \( r_0 \) is shown in Figures 3.2 and 3.3 respectively. For this case of a circular geometry and \( E_+ \) and \( E_- \) data, I have simulation results from calculating the linear in \( E \) shift using \( \frac{d\phi}{dt} \) within ComSol and using Matlab to fit spin time series for their frequencies.
Figure 3.2 Comsol vs Barabanov Data for no gas collisions which is consistent with the conditions in the simulations.

Figure 3.3 Comsol vs Barabanov Data with gas collisions for various $r_0$ values. The numerical data is closest with the simulation data for $r_0 = 0.005$. 
For the numerical integration, the solver can encounter singularities which I handle by using a small $\epsilon$ added to the denominator of Equation 3.15: $[\sin(\delta_0 - \alpha)\sin(\delta_0 + \alpha) + \epsilon]$. As noted in Figure 3.2’s caption, the adiabatic and non-adiabatic limits matched well between my data and the numerical data. But clearly the numerical data including gas collisions matched much better for $r_0 = 0.01$ and $r_0 = 0.005$. For $r_0 = 0.005$, that’s a setup where the mean free path is 200 times larger than the radius of the cylinder. What can also be seen is that when $r_0$ gets too small, the numerical data with gas collisions starts faltering where the no gas collision data did.

### 3.2.2 Comsol Data vs Pignol Theoretical Data

The Pignol, Guigue, Petukhov and Golub paper [GP15] determined universal expressions for frequency shifts in the adiabatic and non-adiabatic limits. These regimes correspond to when $\omega_0 \tau_w >> 1$ and when $\omega_0 \tau_w << 1$ respectively. The paper integrates through correlation functions to determine leading order terms for frequency shifts. For reference, the results summarized in Table 1 of that paper are shown in Table 3.1 below.

**Table 3.1** Various leading term frequency shift expressions from [GP15]

<table>
<thead>
<tr>
<th>Frequency Shift</th>
<th>Adiabatic Limit (UCNs)</th>
<th>Non-Adiabatic Limit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\delta \omega_{B^2}$</td>
<td>$\frac{\tau}{\tau_0} b_z^2 + b_y^2$</td>
<td>$\frac{\tau}{\tau_0} \omega_0 \int_0^\infty \tau &lt; b_x(0) b_x(\tau) + b_y(0) b_y(\tau) &gt; d\tau$</td>
</tr>
<tr>
<td>$\delta \omega_{E^2}$</td>
<td>$\frac{\tau}{\tau_0} &lt; v^2 &gt;$</td>
<td>$-\frac{\tau}{2\tau_0} \omega_0 &lt; x^2 + y^2 &gt;$</td>
</tr>
<tr>
<td>$\delta \omega_{B E}$</td>
<td>$-\frac{\tau}{\tau_0} \frac{\tau}{\tau_0} \left( &lt; \frac{b_z}{x} v_x^2 &gt; + &lt; \frac{b_y}{y} v_y^2 &gt; \right)$</td>
<td>$\frac{\tau}{\tau_0} &lt; b_x x + b_y y &gt;$</td>
</tr>
</tbody>
</table>

#### 3.2.2.1 Circle Simulations

A few things to note about Table 3.1:
- The expressions are assuming three dimensions, ie. $< v_x^2 > = < v_y^2 > = < v_z^2 > = \frac{1}{3} < v^2 >$ but in my two dimensional cell for a cylinder at a constant $z$, $< v_x^2 > = < v_y^2 > = \frac{1}{2} < v^2 >$. And in my simulations, $< v^2 > = 25$ m/s while $v_x$ and $v_y$ vary.
- For a circle, $< x^2 + y^2 > = \frac{R^2}{2}$.
- The $B^2$ non-adiabatic shift cannot be reduced to an analytic expression so I did not do comparisons for it. Also, the non-adiabatic linear in $E$ shift is constant so only useful for my lowest magnetic fields.
- Lastly, for linear and cylindrical symmetric gradients, $b_x = G_x x$ and $b_y = G_y y$; $G_x = G_y = -\frac{G_z}{2}$.

When checking if I was sufficiently in a limit, I decided to use $\alpha = \frac{\pi}{4}$. The plots below show my circle simulation data in blue and Pignol theory in orange. All simulations were done in the rotating frame and I calculated $\frac{d\phi}{dt}$ within ComSol. For the following plots, the non-adiabatic simulations used
Figure 3.4 Simulations in a circle with specular wall collisions using $+E$ and $-E$ to extract a false edm shift.

$$B_0 = (1.35, 2.50, 4.0, 7.0, 8.5, 9.5, 13.5) \cdot 10^{-5} \text{G}$$

$$E = 19.25 \text{ Statvolt/cm, } G_z = 9.004 \cdot 10^{-8} \text{ G/cm}$$

$$R = 20 \text{ cm, } v = 1400 \text{ cm/s.}$$ (3.17)

And for the adiabatic simulations

$$B_0 = (4.05, 7.50, 12.0, 21.0, 25.5, 28.5, 40.5) \cdot 10^{-3} \text{G}$$

$$E = 16200 \text{ Statvolt/cm, } G_z = 2.70 \cdot 10^{-6} \text{ G/cm}$$

$$R = 200 \text{ cm, } v = 500 \text{ cm/s.}$$ (3.18)
Figure 3.5 Simulations in a circle with diffuse scattering wall collisions using $+E$ and $-E$ to extract a false edm shift.

Figure 3.6 Simulations in a circle with diffuse scattering wall collisions using $\frac{d\phi}{dt}$ with G=0.
Figure 3.7 Simulations in a circle with specular wall collisions using $d\phi/dt$ with $G=0$.

The reason there are only four plots instead of ten is because the ComSol data not shown were not matching theory well. Even with the false edm shifts and $E^2$ shifts shown matching pretty well, with deviations less than 1%, I decided to try the simulations in a different geometry: a rectangle.

### 3.2.2.2 Rectangle Simulations

For the rectangular trap, Pignol’s expressions were general so I will compare ComSol data to theoretical expressions just like for the circle. I worked in the dimensionful non-rotating frame and only specular wall collision. With $\vec{v}=5 \text{ m/s}$, I controlled what regime I was in with the strength of the magnetic field as well as the size of the cell. The rectangle was on its ‘side’ so the width was horizontal and longer than the height. For the non-adiabatic regime, I used $w=50 \text{ cm}$, $h=20 \text{ cm}$. For the adiabatic regime, I used $w=200 \text{ cm}, h=100 \text{ cm}$. For a rectangle, there is no radius and while a paper by Steyerl used $1/8$ the perimeter as the radius, I simply used the height which was close to $1/8$ the perimeter. For the non-adiabatic limit, the parameters were

$$B_0 = (1.0, 2.0, 3.0, 8.0, 10.0, 12.3, 15.0, 17.7, 21.8, 26.6, 29.3, 32.1, 34.8) \cdot 10^{-4} \text{ G}$$

$$E = 200 \text{ Statvolt/cm}, \quad G_z = 3.0 \cdot 10^{-7} \text{ G/cm}$$

Equation (3.19)

$$R = 20 \text{ cm}, \quad v = 500 \text{ cm/s}.$$ 

And for the adiabatic simulations

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\[ B_0 = (1.23, 1.50, 1.77, 2.18, 2.66, 2.93, 3.21, 3.48, 4.0, 5.0, 6.0, 7.5, 9.0, 10) \cdot 10^{-3} \text{G} \]

\[ E = 200 \text{ Statvolt/cm}, \quad G_z = 3.0 \cdot 10^{-7} \text{ G/cm} \]

\[ R = 100 \text{ cm}, \quad v = 500 \text{ cm/s}. \] 

(3.20)

**Figure 3.8** Linear in E, false edm shift for a rectangle in the non-adiabatic limit and away from it. The spike in ComSol data after \( \omega' = 1 \) is expected and demonstrates no longer being in the non-adiabatic limit.
Figure 3.9 $E^2$ frequency shift for a rectangle in the non-adiabatic limit and away from it. Again, the large deviation between the data after $\omega' = 1$ is expected and demonstrates no longer being in the non-adiabatic limit.

Figure 3.10 Linear in $E$, false edm shift for a rectangle in the adiabatic limit.
The rectangle simulations matched up quite well with Pignol’s analytic expressions. The differences for the two data sets across plots converge as the limits become more appropriate. ComSol is demon-
strating that solving the Bloch equations for spin components using thousands of random particle trajectories shows agreements with theory.
4.1 Spin Dressing Theory

4.1.1 Lifting the Degeneracy

Understanding the dynamics of spin dressing in regards to the nEDM experiment is crucial for reliable measurements at never before reached sensitivites. From the Golub, Lamoreaux Physics Reports paper \[\text{Gol94}\], the Hamiltonian in Equation 4.1 contains everything I need for a basic spin dressing framework.

Given a spin 1/2 particle in a static magnetic field $B_0$ along $+z$ and an oscillating magnetic field along $x$ with frequency $\omega$, the quantized Hamiltonian is

$$H = \omega a^*a + \gamma \sqrt{2\pi \hbar \omega} s_x (a + a^*) + \omega_0 s_z,$$

(4.1)

where $\gamma$ is the gyromagnetic ratio of the particle and $\omega_0 = -\gamma B_0$. I will treat the last term in Equation 4.1, the static field term, as a perturbation. The Hamiltonian can be transformed \[\text{Pol65}\] such that the unperturbed eigenstates can be defined as

$$|n, m_x\rangle = e^{-(\eta s_x/\omega)(a^*-a)} |n\rangle |m_x\rangle = e^{-(\eta m_x/\omega)(a^*-a)} |n\rangle |m_x\rangle = |n m_x\rangle |m_x\rangle,$$

(4.2)

where $|m_x\rangle$ is an eigenstate of $s_x$ with eigenvalue $m_x$ and for a spin 1/2 particle, $m_x = \pm 1/2$. I will express $|m_x\rangle$ states at $|+\rangle_x$ or $|-\rangle_x$. $|n\rangle$ is an eigenstate of $a^*a$ with eigenvalue $n$. $\eta = \gamma \sqrt{2\pi \hbar \omega}/L^3$ and its definition starts from the energy density of the magnetic field $B_1^2/2 = 4\pi n \hbar \omega /L^3 = 2n \eta^2 /\gamma^2$ such that $\omega_1^2 = 4n \eta^2$ where $\omega_1 = \gamma B_1$.

After transformation, the energy eigenvalues present themselves as
\[ E_{n,m_x} = n \omega - \frac{m_x^2 \eta^2}{\omega}. \] (4.3)

Given the Hamiltonian is now in a transformed state, any expectation values will require calculation of the inner product of two bare states \( \left\langle (n-q)_{1/2} | n_{-1/2} \right\rangle \) which originally done in [Pol65], goes as

\[ e^{\eta/\omega (a^* - a)} e^{-\eta s/2 \omega^2} \approx e^{\eta/\omega a^*} e^{-\eta s/2 \omega^2} \]

\[ -\left\langle n-q \right| \left( \sum_m \left( \frac{n a^*}{\omega} \right)^m \frac{1}{m!} \right) \left( \sum_s \left( \frac{-n a}{\omega} \right)^s \frac{1}{s!} \right) |n\rangle, \]

and from applying the creation and annihilation operators, you can see the only non-zero result is when \( n-q-m=n-s \) so that \( m=s-q \). Assume \( n >> q, s \) and \( n, n-q >> \omega_1 \omega \). Then

\[ \sum_s \left( n-q \right| (-1)^s \left( \frac{n}{\omega} \right)^{2s-q} \left( \frac{a^*}{s-q} \right)^{s-q} a^s \right) \approx \sum_s \left( (-1)^s \left( \frac{n}{\omega} \right)^{2s-q} \left( \frac{s-q}{s} \right)^{s-q} \right) \frac{1}{s!} \]

\[ = J_{-q} \left( 2n \sqrt{\frac{n}{\omega}} \right) = J_{-q} \left( \omega_1 / \omega \right) \]

where \( q = n-n' \), \( J_q(x) \) is the Bessel function of the first kind of order \( q \), I substituted \( \eta = \omega_1 / 2 \sqrt{n} \) and a similar calculation for \( \left\langle n_{1/2} | (n-q)_{-1/2} \right\rangle \) with a result of \( J_q(\omega_1 / \omega) \). Changing the positions of +1/2 or -1/2 changes the sign of the argument.

For a fixed \( n \), the unperturbed states are degenerate in \( m_x \) so I want to calculate the matrix elements from the perturbation \( \omega_0 s_z \) to lift the degeneracy. I diagonalize this matrix in the \( x \) basis to find the eigenvalues and eigenvectors. The sub-matrix elements for a constant \( n \) \((q=0)\) are

\[ \left\langle m'_x, n | \omega_0 s_z | n, m_x \right\rangle = \left\langle m'_x | s_z | m_x \right\rangle \left\langle n_{m'_x} | n_{m_x} \right\rangle \omega_0 \]

\[ = \left\langle m'_x | s_z | m_x \right\rangle \langle n | e^{i m_x s_z} | n_{m'_x} | n_{m_x} \rangle \omega_0 = \frac{\left\langle m'_x | s_z | m_x \right\rangle J_0(m'_x - m_x) \omega_1 / \omega \rangle \omega_0. \]

(4.6)

Given \( s_z = m_z \sigma_z \), I want to solve \( \left\langle m'_x | \sigma_z | m_x \right\rangle \) for all combinations of \( m_x = \pm 1 \) and \( m'_x = \pm 1 \). Writing \( \sigma_z = -i |+\rangle_x \langle + | + | -\rangle_x \langle - | \) (still in \( x \) basis), I have

\[ \pm \langle \pm | \sigma_z | \pm \rangle_x = 0 \]

\[ x \langle | \sigma_z | + \rangle_x = x \langle + | \left[ -i |+\rangle_x \langle + | -i | -\rangle_x \langle - | \right] + \rangle_x = -i \]

\[ x \langle - | \sigma_z | + \rangle_x = x \langle - | \left[ -i |+\rangle_x \langle + | -i | -\rangle_x \langle - | \right] + \rangle_x = i \]

so that the matrix I must diagonalize is

\[ x \langle | \sigma_z | + \rangle_x = \]

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\[
\frac{1}{2} \omega_0 \begin{pmatrix}
0 & -i J_0(\omega_1/\omega) \\
 i J_0(-\omega_1/\omega) & 0
\end{pmatrix}.
\] (4.8)

The eigenvalues come from the determinant after inserting \(-\lambda\)'s such that the eigenvalue equation and its solution is

\[
\lambda^2 - J_0(\omega_1/\omega)J_0(-\omega_1/\omega) \frac{1}{4} \omega_0^2 = 0 \\
\lambda = \pm \frac{1}{2} J_0(\omega_1/\omega) \omega_0 \equiv m_z \omega_d.
\] (4.9)

Equation 4.9 shows by how much the energy levels are shifted. Solving for the eigenvectors \( \vec{k}_1 \) and \( \vec{k}_2 \)

\[
\frac{\omega_0}{2} \begin{pmatrix}
J_0(\omega_1/\omega) & -i J_0(\omega_1/\omega) \\
i J_0(\omega_1/\omega) & J_0(\omega_1/\omega)
\end{pmatrix} \vec{k}_1 = 0 \\
\vec{k}_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} i \\ 1 \end{pmatrix}
\] (4.10)

\[
\frac{\omega_0}{2} \begin{pmatrix}
-J_0(\omega_1/\omega) & -i J_0(\omega_1/\omega) \\
 i J_0(\omega_1/\omega) & -J_0(\omega_1/\omega)
\end{pmatrix} \vec{k}_2 = 0 \\
\vec{k}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} -i \\ 1 \end{pmatrix}
\]

\[
\vec{k}_1 = \frac{1}{\sqrt{2}}(|+\rangle_x + i |-\rangle_x) \\
\vec{k}_2 = \frac{1}{\sqrt{2}}(|+\rangle_x - i |-\rangle_x)
\] (4.11)

The Physics Reports [Gol94] has the \( m_z \) eigenstates as

\[
|n, m_z\rangle = \frac{1}{\sqrt{2}}(|n_+\rangle |+_\rangle_x + i m_z |n_-\rangle |-_\rangle_x)
\] (4.12)

which is an equivalent form of the eigenvectors in Equation 4.11 for spin along +z and -z \((m_z = \pm 1)\).

Going forward, I will write \( m_z \) as \( m \) and any states with a + or - is a state in the \( x \) basis.

### 4.1.2 Expectation Values

Given Equation 4.12 are eigenstates that lift the degeneracy in the Hamiltonian, I can now derive expressions for spin expectation values. For each component that follows, I will first show the matrix elements using Equation 4.12 and then incorporate the elements into a time dependent wave function.

The matrix elements for \( \sigma_y \) are
\[\langle n', m'|\sigma_y|n, m \rangle = \left(\langle n'_+| + i m'|n'_-| \right) \langle n| + + |n| + + |n| + + i m|n| - - \right) \]
\[= \left( i m|n' + n| - i m'|n'_-|n'_+ \right) = \left( m\langle n - q| + n| - m'|n - q| - n \right) \]
\[= i \left( m J_{-q}(\omega_1/\omega) - m' J_q(\omega_1/\omega) \right) = i \left( m J_q(\omega_1/\omega)(-1)^q - m' J_q(\omega_1/\omega) \right), \tag{4.13}\]
so that the expectation value is
\[<\sigma_y(t)> = \sum_{m,q} \sum_{n,n'} \frac{1}{2} a_n^* a_n e^{-in'\omega t} e^{-im'\omega dt/2} i \left( m J_q(\omega_1/\omega)(-1)^q - m' J_q(\omega_1/\omega) \right) e^{im'\omega dt/2} e^{in\omega t}. \tag{4.14}\]
a_n are Glauber coefficients which describe the probability amplitudes of photons of a harmonic field. They can be expressed as
\[a_n = e^{-\eta/2} \frac{\eta^{n/2}}{(n!)^{1/2}}, \tag{4.15}\]
where \(\eta = <n>\), the average photon number. Then for large \(n\), \(\sum_n |a_n|^2 = 1\). Given selection rules on \(m\) and \(m'\) and summing over these values, the expectation value for \(\sigma_y\) becomes
\[<\sigma_y(t)> = \sum_{m,q} \frac{1}{2} e^{iq\omega t} e^{-i(2m' - m)\omega dt} i \left( m J_q(\omega_1/\omega)(-1)^q - m' J_q(\omega_1/\omega) \right) \]
\[= -J_0(\omega_1/\omega) \sin \omega dt - \sum_{q > 0, even} J_q(\omega_1/\omega) \left[ \sin(\omega dt + q \omega t) + \sin(\omega dt - q \omega t) \right]. \tag{4.16}\]

For \(\sigma_z\)
\[\langle n', m'|\sigma_z|n, m \rangle \]
\[= \left(\langle n'_+| + - i m'|n'_-| \right) \langle n| + - i + |n| + + i m|n| - - \right) \]
\[= \left( m J_{-q}(\omega_1/\omega) + m' J_q(\omega_1/\omega) \right) = \left( m J_q(\omega_1/\omega)(-1)^q + m' J_q(\omega_1/\omega) \right). \tag{4.17}\]
So that the expectation value is
\[<\sigma_z(t)> = \sum_{m,q} \sum_{n,n'} \frac{1}{2} a_n^* a_n e^{-i(n' - n)\omega t} e^{-i(2m' - m)\omega dt} \left( m J_q(\omega_1/\omega)(-1)^q + m' J_q(\omega_1/\omega) \right) \]
\[= \sum_{m,q} \frac{1}{2} e^{iq\omega t} e^{-i(2m' - m)\omega dt} \left( m J_q(\omega_1/\omega)(-1)^q + m' J_q(\omega_1/\omega) \right) \]
\[= \sum_{q > 0, odd} J_q(\omega_1/\omega) \left[ \cos(\omega dt - q \omega t) - \cos(\omega dt + q \omega t) \right]. \tag{4.18}\]
And finally, for \(\sigma_x\)
\[ \langle n', m' | \sigma_z | n, m \rangle = (\langle n'_+ | (+) - i m' \langle n'_- | (-) \rangle (+) + (-) \langle n'_- | +i m | n'_+ \rangle (-) \rangle ) = \delta_{n,n'} \left( J_0(0) - m' J_0(0) \right) = \delta_{n,n'} (1 - m' m). \]  

(4.19)

So that the expectation value is

\[
\langle \sigma_x(t) \rangle = \sum_{m,n'} \sum a^*_n a_n e^{-i m' \omega t} e^{-i m' \omega t/2} \delta_{n,n'} (1 - m' m) e^{i \omega t} e^{i \omega t t/2} 
\]

(4.20)

Thus, I have expressions for how spin expectations values evolve through time. When it comes to my simulation work, the comparison of simulation data versus these expressions is important to benchmark the simulations before extending them to higher complexities. After making a fourth order Runge-Kutta (RK4) solver in Matlab to solve the spin Bloch equations, I saw there were frequencies matching with theory as well as additional frequencies which have not been accounted for in the Physics Reports. I then saw confluence of the RK4 results with the near-exact Hamiltonian method.

4.2 The 4th Order Runge-Kutta Solver for Spin Bloch Equations

4.2.1 Constructing the Solver

The spin Bloch equations can be easily solved in Matlab by constructing a fourth-order Runge-Kutta solver. Given these Bloch equations

\[
\frac{d \vec{S}}{dt} = \gamma (\vec{S} \times \vec{B}),
\]

(4.21)

I can specify field parameters, time steps, simulation time and initial conditions as inputs into my RK4. The paragraph below this one shows the initialization of the Bloch equations as differential equations within Matlab as well as initial conditions. BxN, ByN and BzN refers to the total magnetic field components for all particles N. The gamma(s) refers to whether I will be using \( \gamma_3 \) or \( \gamma_n \) for \( s = 1 \) or \( s = 2 \) respectively. The inner most ‘for loop’ loops through \( s = 1 \) for simulations of \(^3\text{He}\) and then UCN’s. The difference between initial==0, 1 is whether the \(^3\text{He}\) and UCN are initially parallel or perpendicular.

\[
dSxdt = @(Sy,Sz,ByN,BzN) (Sy*BzN-Sz*ByN)*gamma(s); \\
dSydt = @(Sx,Sz,BxN,BzN) (Sz*BxN-Sx*BzN)*gamma(s); \\
dSzdt = @(Sx,Sy,BxN,ByN) (Sx*ByN-Sy*BxN)*gamma(s); \\
\]

%initial conditions
if initial == 0
    if s == 1

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Sx(:,1)=0; Sy(:,1)=1; Sz(:,1)=0;
end
if s == 2
    Sx(:,1)=1; Sy(:,1)=0; Sz(:,1)=0;
end
end
if initial == 1
    Sx(:,1)=1; Sy(:,1)=0; Sz(:,1)=0;
end

The next paragraph shows the actual RK4 looping through all time steps within a loop through all particles. What’s interesting to note in the k coefficients is that the fields use time steps 1/2 those used in the spins. For spin dressing with a static field, it’s easy to implement fields that have half the time step of what the spins will be. However, when it comes to incorporating gradients and electric fields for magnetic fields depend on trajectories, what’s needed is purposely halving the time steps in Comsol so that the trajectories construct appropriate magnetic fields.

for M=1:N
    for i=1:tn-1
        k1x = dSxdt(Sy(M,i),Sz(M,i),ByN(M,2*i-1),BzN(M,2*i-1));
        k1y = dSydt(Sx(M,i),Sz(M,i),BxN(M,2*i-1),BzN(M,2*i-1));
        k1z = dSzdt(Sx(M,i),Sy(M,i),BxN(M,2*i-1),ByN(M,2*i-1));

        k2x = dSxdt(Sy(M,i)+h/2*k1y,Sz(M,i)+h/2*k1z,ByN(M,2*i),BzN(M,2*i));
        k2y = dSydt(Sx(M,i)+h/2*k1x,Sz(M,i)+h/2*k1z,BxN(M,2*i),BzN(M,2*i));
        k2z = dSzdt(Sx(M,i)+h/2*k1x,Sy(M,i)+h/2*k1y,BxN(M,2*i),ByN(M,2*i));

        k3x = dSxdt(Sy(M,i)+h/2*k2y,Sz(M,i)+h/2*k2z,ByN(M,2*i),BzN(M,2*i));
        k3y = dSydt(Sx(M,i)+h/2*k2x,Sz(M,i)+h/2*k2z,BxN(M,2*i),BzN(M,2*i));
        k3z = dSzdt(Sx(M,i)+h/2*k2x,Sy(M,i)+h/2*k2y,BxN(M,2*i),ByN(M,2*i));

        k4x = dSxdt(Sy(M,i)+h*k3y,Sz(M,i)+h*k3z,ByN(M,2*i+1),BzN(M,2*i+1));
        k4y = dSydt(Sx(M,i)+h*k3x,Sz(M,i)+h*k3z,BxN(M,2*i+1),BzN(M,2*i+1));
        k4z = dSzdt(Sx(M,i)+h*k3x,Sy(M,i)+h*k3y,BxN(M,2*i+1),ByN(M,2*i+1));

        Sx(M,i+1) = Sx(M,i)+h/6*(k1x + 2*k2x + 2*k3x + k4x);
        Sy(M,i+1) = Sy(M,i)+h/6*(k1y + 2*k2y + 2*k3y + k4y);
        Sz(M,i+1) = Sz(M,i)+h/6*(k1z + 2*k2z + 2*k3z + k4z);
Additionally, I also created an RK5 solver which can be seen in Appendix A1 and given the time steps required for the fields, it's clearly not practical for fields that need trajectories from ComSol. Moreover, I saw no benefit in accuracy when testing the RK4 vs the RK5 for simple cases while the RK5 took substantially longer to solve. Therefore, I will use solely the RK4 going forward. The results of the RK4 are spins of size \(N \times \frac{1}{\text{tstep}} + 1\) that can be ensemble averaged for the spin time series that represent the system. A more complete script for my RK4 is shown below.

```matlab
for xmp = 1:length(xm1)
    for xmn = 1:length(xm2)
        for s=1:2 % s switches between He and ucn
            Bo = 3*10^-6; y = 1/10;
            Gz = 0;
            E = 0; %Bo/10^-14*(-1)^s; %Bo*c^2/100/vo*(-1)^s;
            Gx = -Gz/2; Gy = -Gz/2;
            wo(s) = -Bo*gamma(s);
            P = 1*10^-9*pseudo_off_on;

            w = -Bo*gamma(2)/y;
            Brf = (xc)*w/gamma(2);
            xn = gamma(2)*Brf/w; x3 = gamma(1)*Brf/w;
            wn = besselj(0,xc)*-Bo*gamma(2);
            w3 = besselj(0,alpha*xc)*-Bo*gamma(1);

            Brf1 = (xc+xm1(xmp))*w/gamma(2);
            Brf2 = (xc-xm2(xmn))*w/gamma(2);
            w1 = Brf/(xc+xm1(xmp))*gamma(2);
            w2 = Brf/(xc-xm2(xmn))*gamma(2);

            % create modulation Brf fields. Alternate applying. f_m = intervals/T

            L = Lt2-1;
            if Bd_mod_off_on == 0
                Bd = Brf*cos(w*t2);
            end
            if Bd_mod_off_on == 1

```

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for i=1:intervals+1  %%This interval loop only works for >5 intervals
  if i==1  %%start with tau/2
    Bd(1,1:L/(2*intervals)) = Brf1*cos(w*t2(1:L/(2*intervals)));  
  end
  if i == 2  %%tau +wz right after tau/2 interval
    Bd(1,L/(2*intervals)+1:L/(2*intervals)+(i-1)*L/(intervals))
    = Brf2*cos(w*t2(L/(2*intervals)
               +1:L/(2*intervals)+(i-1)*L/(intervals)));  
  end
  if i > 2 && i < intervals+1 && mod(i,2) == 1  %%tau -wz
    Bd(1,L/(2*intervals)+(i-2)*L/(intervals)
        +1:L/(2*intervals)+(i-1)*L/(intervals))
    = Brf1*cos(w*t2(1,L/(2*intervals)+(i-2)*L/(intervals)
                   +1:L/(2*intervals)+(i-1)*L/(intervals)));  
  end
  if i > 2 && i < intervals+1 && mod(i,2) == 0  %%tau +wz
    Bd(1,L/(2*intervals)+(i-2)*L/(intervals)
        +1:L/(2*intervals)+(i-1)*L/(intervals))
    = Brf2*cos(w*t2(1,L/(2*intervals)+(i-2)*L/(intervals)
                   +1:L/(2*intervals)+(i-1)*L/(intervals)));  
  end
  if i == intervals+1  %%tau/2 -wz (intervals = even causes tau/2 -wz at end)
    Bd(1,L-L/(2*intervals)+1:L+1)
    = Brf1*cos(w*t2(L-L/(2*intervals)+1:L+1));  
  end
end

Bx = zeros(N,length(t2)); By = zeros(N,length(t2)); Bz = Bo+zeros(N,length(t2));

%Create Bx, By, Bz row vectors corresponding to each particle

BxN = zeros(N,tn);
ByN = zeros(N,tn);
BzN = zeros(N,tn);

%For dressing field, add each element of Bd at each time to each element of
%BxN, particle by particle
for i=1:N 
  for n=1:tn*2-1 
    BxN(i,n) = Bx(n*N-N+i);
    ByN(i,n) = By(n*N-N+i);
    BzN(i,n) = Bz(n*N-N+i);
  end
end
%spin dressing
    BxN(i,:) = BxN(i,:) + Bd(1,:);
%pseudo mag field
    if s==2
        BxN(i,:) = BxN(i,:) + Px(1,:);
        ByN(i,:) = ByN(i,:) + Py(1,:);
        BzN(i,:) = BzN(i,:) + Pz(1,:);
    end
end

Sx = zeros(N,tn);
Sy = zeros(N,tn);
Sz = zeros(N,tn);

%Define functions representing each differential equation that’ll be
%approximated with RK4

dSxdt = @(Sy,Sz,ByN,BzN) (Sy*BzN-Sz*ByN)*gamma(s);
dSydt = @(Sx,Sz,BxN,BzN) (Sz*BxN-Sx*BzN)*gamma(s);
dSzdt = @(Sx,Sy,BxN,ByN) (Sx*ByN-Sy*BxN)*gamma(s);

%initial conditions
    if initial == 0
        if s == 1
            Sx(:,1)=0; Sy(:,1)=1; Sz(:,1)=0;
        end
        if s == 2
            Sx(:,1)=1; Sy(:,1)=0; Sz(:,1)=0;
        end
    end
    if initial == 1
        Sx(:,1)=1; Sy(:,1)=0; Sz(:,1)=0;
    end

n = T/h;
%calculate each k

for M=1:N
    for i=1:tn-1
        k1x = dSxdt(Sy(M,i),Sz(M,i),ByN(M,2*i-1),BzN(M,2*i-1));
        k1y = dSydt(Sx(M,i),Sz(M,i),BxN(M,2*i-1),BzN(M,2*i-1));
        k1z = dSzdt(Sx(M,i),Sy(M,i),BxN(M,2*i-1),ByN(M,2*i-1));

        k2x = dSxdt(Sy(M,i)+h/2*k1y,Sz(M,i)+h/2*k1z,ByN(M,2*i),BzN(M,2*i));
        k2y = dSydt(Sx(M,i)+h/2*k1y,Sz(M,i)+h/2*k1z,BxN(M,2*i),ByN(M,2*i));
        k2z = dSzdt(Sx(M,i)+h/2*k1y,Sy(M,i)+h/2*k1z,BxN(M,2*i),ByN(M,2*i));

        k3x = dSxdt(Sy(M,i)+h/2*k2y,Sz(M,i)+h/2*k2z,ByN(M,2*i),BzN(M,2*i));
        k3y = dSydt(Sx(M,i)+h/2*k2y,Sz(M,i)+h/2*k2z,BxN(M,2*i),ByN(M,2*i));
        k3z = dSzdt(Sx(M,i)+h/2*k2y,Sy(M,i)+h/2*k2z,BxN(M,2*i),ByN(M,2*i));

        k4x = dSxdt(Sy(M,i)+h/2*k3y,Sz(M,i)+h/2*k3z,ByN(M,2*i),BzN(M,2*i));
        k4y = dSydt(Sx(M,i)+h/2*k3y,Sz(M,i)+h/2*k3z,BxN(M,2*i),ByN(M,2*i));
        k4z = dSzdt(Sx(M,i)+h/2*k3y,Sy(M,i)+h/2*k3z,BxN(M,2*i),ByN(M,2*i));

        Sx(M,i+1) = Sx(M,i) + h/6*(k1x + 2*k2x + 2*k3x + k4x);
        Sy(M,i+1) = Sy(M,i) + h/6*(k1y + 2*k2y + 2*k3y + k4y);
        Sz(M,i+1) = Sz(M,i) + h/6*(k1z + 2*k2z + 2*k3z + k4z);
    end
end
k2y = dSydt(Sx(M,i)+h/2*k1x,Sz(M,i)+h/2*k1z,BxN(M,2*i),BzN(M,2*i));
k2z = dSzdt(Sx(M,i)+h/2*k1x,Sy(M,i)+h/2*k1y,BxN(M,2*i),ByN(M,2*i));

k3x = dSxdt(Sy(M,i)+h/2*k2y,Sz(M,i)+h/2*k2z,BxN(M,2*i),BzN(M,2*i));
k3y = dSydt(Sx(M,i)+h/2*k2x,Sz(M,i)+h/2*k2z,BxN(M,2*i),BzN(M,2*i));
k3z = dSzdt(Sx(M,i)+h/2*k2x,Sy(M,i)+h/2*k2y,BxN(M,2*i),ByN(M,2*i));

k4x = dSxdt(Sy(M,i)+h*k3y,Sz(M,i)+h*k3z,BxN(M,2*i+1),BzN(M,2*i+1));
k4y = dSydt(Sx(M,i)+h*k3x,Sz(M,i)+h*k3z,BxN(M,2*i+1),BzN(M,2*i+1));
k4z = dSzdt(Sx(M,i)+h*k3x,Sy(M,i)+h*k3y,BxN(M,2*i+1),ByN(M,2*i+1));

Sx(M,i+1) = Sx(M,i)+h/6*(k1x + 2*k2x + 2*k3x + k4x);
Sy(M,i+1) = Sy(M,i)+h/6*(k1y + 2*k2y + 2*k3y + k4y);
Sz(M,i+1) = Sz(M,i)+h/6*(k1z + 2*k2z + 2*k3z + k4z);

SxTot(s,:) = Sx;
SyTot(s,:) = Sy;
SzTot(s,:) = Sz;

x_eff = xc*alpha_list(s);
wd = wo(s)*besselj(0,x_eff)
-wd(s)*alpha_list(s)^2*besselj(0,x_eff)*y^2/2*(3*besselj(1,x_eff)^2/besselj(2,x_eff)^2/4+3*besselj(3,x_eff)^2/9);

%Fitting Sx
if fit_off_on == 1
[xData,yData] = prepareCurveData(t,SxTot(s,:));

ft = fittype( 'a*cos(b*x+c)' , 'independent' , 'x' , 'dependent' , 'y' );
opts = fitoptions( 'Method' , 'NonlinearLeastSquares' );
opts.Display = 'Off';
opts.Lower = [0.99 wd-5 -4];
opts.StartPoint = [1 wd 0];
opts.Upper = [1.01 wd+5 4];

% Fit model to data.
[fitresult, gof] = fit( xData, yData, ft, opts );
coeffs = coeffvalues(fitresult);
weff(s) = coeffs(2);
Rsquared_list = [Rsquared_list, gof.rsquare];
end

% solve for He spin vector angles to align pseudo mag field

polar_he = acos(SzTot(1,:));
azimuthal_he = acos(SxTot(1,:)./(sin(polar_he)));

for i=1:length(polar_he)
    Px(1,2*i-1) = P*cos(azimuthal_he(1,i)).*sin(polar_he(1,i));
    Py(1,2*i-1) = P*sin(azimuthal_he(1,i)).*sin(polar_he(1,i));
    Pz(1,2*i-1) = P*cos(polar_he(1,i));
end

for i=1:length(t2)
    if mod(i,2) == 0
        Px(1,i) = (Px(1,i-1)+Px(1,i+1))/2;
        Py(1,i) = (Py(1,i-1)+Py(1,i+1))/2;
        Pz(1,i) = (Pz(1,i-1)+Pz(1,i+1))/2;
    end
end
end

weff_diff(xmp,xmn) = weff(1)-weff(2);
weff_sum(xmp,xmn) = weff(1)+weff(2);

phase_diff_from_fit(xmp,xmn) = T*(weff(1)-weff(2));

Bs = [Bs,Bo];

Sx_he_ucn = SxTot(1,:).*SxTot(2,:);
Sy_he_ucn = SyTot(1,:).*SyTot(2,:);
Sz_he_ucn = SzTot(1,:).*SzTot(2,:);

S_Tot_he_ucn = Sx_he_ucn+Sy_he_ucn+Sz_he_ucn;
%S_Tot_he_ucn = Sy_he_ucn+Sz_he_ucn;

% 3D plot
if plot_nD == 1
    axis([-1 1 -1 1 -1 1]); axis square
    grid on
    st = 1;
h3 = plot3(SxTot(1,st),SyTot(1,st),SzTot(1,st),'r','LineWidth',1);
hold on
ucn = plot3(SxTot(2,st),SyTot(2,st),SzTot(2,st),'b','LineWidth',1);

for i=st+1:st+1+200000
    set(h3,'xdata',SxTot(1,st:i),'ydata',SyTot(1,st:i),'zdata',SzTot(1,st:i));
    set(ucn,'xdata',SxTot(2,st:i),'ydata',SyTot(2,st:i),'zdata',SzTot(2,st:i));
    pause('off');
end
hold off
end

%2D plot
if plot_nD == 2
    axis([-1 1 -1 1]); axis square
    grid on
    st = 1995000;
    h3 = plot(SxTot(1,st),SyTot(1,st),'r','LineWidth',1);
    hold on
    ucn = plot(SxTot(2,st),SyTot(2,st),'b','LineWidth',1);
    for i = st+1:st+1+5000
        set(h3,'xdata',SxTot(1,st:i),'ydata',SyTot(1,st:i));
        set(ucn,'xdata',SxTot(2,st:i),'ydata',SyTot(2,st:i));
        pause(.000001);
    end
    hold off
end

polar_he = acos(SzTot(1,:));
azimuthal_he = acos(SxTot(1,:)./sin(polar_he));
polar_u = acos(SzTot(2,:));
azimuthal_u = acos(SxTot(2,:)./sin(polar_u));

final_phase_diff(xmp,xmn) = azimuthal_he(1,length(t))-azimuthal_u(1,length(t));
phase_diff_u_he = azimuthal_u - azimuthal_he;

polar_he_mean(xmp,xmn) = pi/2-mean(polar_he);
polar_u_mean(xmp,xmn) = pi/2-mean(polar_u);
polar_he_ucn = acos(S_Tot_he_ucn);
apizimuthal_he_ucn = acos(S_Tot_he_ucn./sin(polar_he_ucn));

polar_he_ucn_mean(xmp,xmn) = mean(polar_he_ucn)-pi/2;

azimuthal_he_ucn_mean = mean(azimuthal_he_ucn);

S_Tot_he_ucn_mean(xmp,xmn) = mean(S_Tot_he_ucn);

end
end

where some of the script is used to fit $\sigma_x$ or plot 2D or 3D curves or align the pseudomagnetic field along the $^3$He.

### 4.2.2 Testing Against Theory

There are many ways to test my RK4 against theory. Two straightforward and relevant ways are to first, apply only a static field along $+z$ with the spins parallel along $+x$ and measure their Larmor frequencies. And second, dress the spins and compare the results to expectation values from the previous section - specifically, whether $\omega_0$ gets a factor of $J_0(x)$ on it. What is very convenient is due to these simulations only containing fields independent of trajectories, I can use only one particle: $N = 1$.

For the first test, $B_0 = 3 \cdot 10^{-6}$ T, I run the simulation and fit the $\sigma_x$ for the two particles. I use Matlab’s ’prepareCurveData’ and ’fittype’ functions to fit a $a \cdot \cos(b \cdot t + c)$ function to the data. I can specify lower and upper ranges and a start point for the fitting to more efficiently find the best values. I can also record the $R^2$’s for any fit to make sure the fit is sufficiently accurate. The test results are

$$\omega_{03} = 611.3576 \text{ rad/s}, \quad \omega_{0n} = 549.7415 \text{ rad/s}$$

$$\omega_{03} - \omega_{0n} = 61.6160 = (\alpha - 1)\omega_{0n} \text{ rad/s.}$$

The expected results are that $\omega_{0i} = -\gamma_i B_0$ (where $\gamma_i$ is negative). This also means that the difference between the $^3$He and neutron Larmor frequency will simply be $(\alpha - 1)\omega_{0n}$. Equation 4.22 shows the RK4 has given results matching theory. For the next test, I’ll use the following parameters

$$B_0 = 3 \cdot 10^{-6}, \quad y = 0.10, \quad x_c = 1.1824619208064$$

$$\omega = -B_0\gamma_n/y$$

$$B_{rf} = x_c \omega/\gamma_n,$$

where the $x_c$ was determined through trial and error by looping through many values of x and finding the value that led to the lowest difference between dressed $\omega_{03}$ and dressed $\omega_{0n}$ which was on the order of $10^{-12}$ rad/s. Going forward, the dressed Larmor frequencies will be written as $\omega_3$ and $\omega_n$. The results are
\[
\omega_3 = \omega_n = 372.5987 \text{ rad/s} \\
\approx \omega_0 J_0(x_c) \approx \omega_0 \alpha J_0(\alpha x_c).
\] (4.24)

Equation 4.24 shows that the RK4 solver being used in a spin dressing environment is producing an approximately correct shift to the Larmor frequency since the first order correction to the eigenvalues that I solved for earlier in this chapter are indeed diluting the Larmor frequencies. The reason the results aren't more accurate are made clear in the next chapter.

Another test is whether \(\frac{\pi}{2}\) and \(\pi\) pulses with no spin dressing properly rotate the spins. So this would be a setup with a static field accompanied by a weak alternating field on resonance and only present during the pulse duration. To mimic the experiment, I will start with the spins aligned along +\(z\). I will apply a \(\frac{\pi}{2}\) pulse on resonance at \(t = 0.40\text{s}\). And for demonstrating the example further, I'll apply one more \(\frac{\pi}{2}\) pulse at \(t = 1.20\text{s}\). The plots of \(\sigma_x\), a zoomed in view of \(\sigma_x\) at the first pulse time and \(\sigma_z\) for \(^3\text{He}\) are shown in Figures 4.1 and 4.2.
Figure 4.1 $\sigma_x$ for $^3$He initially pointing along $+z$ and $\pi/2$ pulses on resonance applied at $t = 0.40\text{s}$ and $t = 1.2\text{s}$ for a duration of 0.001s.
Figure 4.2 $\sigma_z$ for $^3$He initially point along +z and $\pi/2$ pulses on resonance applied at $t = 0.40s$ and $t = 1.2s$ for a duration of $t_p = 0.001s$.

What can be seen is that $\sigma_x$ has the expected behavior: starts at 0, oscillates between 1 and -1 after the first pulse and goes back to 0 after the second pulse. Whereas $\sigma_z$ starts at 1, goes to 0 after the first pulse and then to -1 after the second pulse.

For one final demonstration of the RK4’s abilities, I will show a spin echo using 1000 particle trajectories from ComSol. The premise of a spin echo is that for T2 dephasing, a pulse that rotates the spins can reverse the dephasing, albeit temporarily. The equations of the fields I’ll use are

$$
\begin{align*}
B_x &= G_x \cdot x + v_y \cdot E / c^2 \\
B_y &= G_y \cdot y - v_x \cdot E / c^2 \\
B_z &= B_0 + G_z \cdot z \\
G_x + G_y + G_z &= 0, G_x = G_y
\end{align*}
$$

(4.25)

where the trap is a cylinder, gradients are linear and have cylindrical symmetry, and $B_0$ and $E$ point along +z. So if the spins start along +z, are rotated to the x-y plane and dephase due to gradients and motional fields, a $\pi$ pulse can flip the spins such that what was dephasing is now ‘rephasing’ temporarily. An example of this is shown in Figure 4.3. A $\pi/2$ pulse is applied at 0.10s for a duration of 0.001s. Relaxation occurs because of the cylindrical gradients and motional field. It is then partially reversed due to a $\pi$ pulse at 0.25s. Then more T2 relaxation takes its course but naturally gets reversed after near maximum dephasing.
4.3 Anomalous Frequencies in Dressed Spins

For my RK4, incorporating spin dressing simply means including it in the net fields used in the Bloch equations. For the study of these spin dressing computations, there's no need for any trajectory data so things are simple. The fields will be

\[ \begin{align*}
B_x(t) &= B_1 \cos \omega t \\
B_y &= 0 \\
B_z &= B_0 \\
y &\equiv \omega_0 / \omega, \quad x \equiv \gamma_3 B_1 / \omega = \omega_1 / \omega.
\end{align*} \tag{4.26} \]

Figure 4.3 $\sigma_x$ with $\vec{\sigma}$ initially pointing along +z. A $\pi/2$ pulse at $t = 0.10$ s brings $\vec{\sigma}$ to +x. Dephasing is a constant due to trajectories sampling gradient and motional fields. A $\pi$ pulse applied at $t = 0.25$ s reverses dephasing to form a spin echo.
Using initial conditions $S_x = 1$, $S_y = 0$ and $S_z = 0$, time steps of $t_{step} = 0.0005$ s for the spin components and $t_{step}/2$ for magnetic field time steps, the RK4 will solve for spins as a function of time. An example of a three dimensional plot for $\textsuperscript{3}$He (red) and UCN (blue) critical dressing is shown in Figure 4.4.

For the rest of this chapter, the simulation time is $T = 10.0$ s and the actual computation can take anywhere from minutes to hours. I will use $N = 1$. Finally, the relevant parameters for the first results I will show are

$$B_0 = 1\text{mG}$$
$$y = 0.10, x = 1.189.$$ (4.27)

The results are spins as a function of time: $\sigma_x(t)$, $\sigma_y(t)$ and $\sigma_z(t)$. I then take the fast Fourier transform of these time series and I can see relevant frequencies. From the theory in the previous section, I expect certain frequencies for each spin component. The plots in Figures 4.5 to 4.7 are the FFTs of the spins for the parameters in Equation 4.27 in light green as well as theory in black. I chose these colors and to have the light green 5% thicker than the black to give contrast between the RK4 results and theory. The time steps are very small and therefore the frequency range is large so the following plots are zoomed in for better inspection of the relevant frequencies.
Figure 4.5 $\sigma_x$ for $y = 0.10$, frequencies solved for using the RK4 method. $\omega$ and $\omega_d \pm 2\omega$ are frequencies not currently included in theory.

Figure 4.6 $\sigma_y$ for $y = 0.10$, frequencies solved for using the RK4 method. $\omega$ and $3\omega$ are frequencies not currently included in theory.
The theory in Figures 4.5 to 4.7 are the predicted results from Equations 4.16, 4.18 and 4.20 in section 4.1.2. I see there are frequencies and harmonics consistent with the expectation values in that section. Furthermore, the ratio of the heights of the expected peaks are in-line with ratios of Bessel function of the first kind of corresponding order amplitudes. But what is quite interesting are the peaks that the theory doesn’t predict. In figure 4.4 for $\sigma_x$, I see these ‘unexpected’ frequencies of $\omega$ and $\omega_d \pm 2\omega$ are almost negligible. But in Figure 4.6 for $\sigma_y$, the unexpected peaks at $\omega$ and $3\omega$ are no longer negligible. And for $\sigma_z$ in Figure 4.7, the unexpected frequencies of $0\omega$ and $2\omega$ have non-negligible intensities.
Figure 4.8 $\sigma_y$ for $y = 0.01$, frequencies solved for using the RK4 method. $\omega$ and $3\omega$ are frequencies not currently included in theory.

Figure 4.9 $\sigma_z$ for $y = 0.01$, frequencies solved for using the RK4 method. $0\omega$ and $2\omega$ are frequencies not currently included in theory.
Figures 4.8 and 4.9 show what Figures 4.4-4.6 showed but for $y = 0.01$ meaning $\omega$ is ten times larger. What’s interesting is that the unexpected frequencies decreased in height substantially between $y = 0.10$ and $y = 0.01$. Given $y$ is a measure of the perturbing static field relative to the rate of oscillation of the dressing field, peak height dependence on $y$ points to missing higher order perturbation theory terms. There is also a ratio of heights strictly between the unexpected peaks that seems to be conserved between the different $y$’s.

The question then is: are these unexpected frequencies due to the RK4 numerical solver issues in Matlab or is it from higher order perturbation theory terms? The reduction in intensity when $y$ is smaller would suggest the latter. Some theoretical models use $y$ anywhere between 0.10 and 0.01 while the experiment will use $y = 0.10$. Figures 4.10 to 4.12 show how these anomalous frequency peaks change as the perturbation strength changes. I chose two frequencies from $\sigma_x (\omega$ and $\omega_d - 2\omega)$ and one each from $\sigma_y (\omega)$ and $\sigma_z (0\omega)$. Then stepped $y$ by 0.0001 between 0.01 and 0.10.

![Graph](image)

**Figure 4.10** $\sigma_x$, $\omega$ heights vs $y$ using the RK4. Intensity ranges from 36.10 to 4031.40.
Figure 4.11 $\sigma_x, \omega_d - 2\omega$ heights vs $y$ using the RK4. Intensity ranges from 369.74 to 4303.59.

Figure 4.12 $\sigma_y$, $\omega$ and $\sigma_z$, $0\omega$ heights vs $y$ using the RK4. Intensity ranges from 4050.20 to 41863.11 and 6860.89 to 68212.28 respectively.

The oscillatory behavior in Figures 4.10 to 4.12 most likely comes from numerical issues within the
solver. From Figure 4.12, the unexpected frequencies I chose from $\sigma_y$ and $\sigma_z$ show $y$ dependence for the $\sigma_y$ and $\sigma_z$ unexpected heights. What’s interesting is that from Figures 4.10 and 4.11, unexpected frequencies for $\sigma_x$ show $y^2$ and $y$ dependence respectively. Going forward, I will call these unexpected frequencies 'anomalies'.

Given the dependence on $y$, the anomalies most likely come from perturbation theory. But even so, the next section shows a different method for solving for expectation values and frequencies of spin components to provide further evidence that the anomalies belong. If it can give confluence to the RK4 method, I will use higher order perturbation theory to more accurately represent this system.

### 4.4 The Hamiltonian Method

#### 4.4.1 Theory

Diagonalizing the Hamiltonian in Equation 4.1 is a method that for high photon number $N_p$, converges towards an exact solution with time to solve as my constraint. For $N_p$ very large, $n$ refers to an addition or subtraction relative to $N_p$. This also mean the $\sqrt{n}$ in $\eta$ can be ignored. Given this Hamiltonian and how the creation and annihilation operators effect adjacent states, the Hamiltonian matrix in the $z$ basis up to $n = \pm 2$ can be written as

\[
\begin{pmatrix}
2 + a & 0 & 0 & b & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 2 - a & b & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & b & 1 + a & 0 & 0 & b & 0 & 0 & 0 & 0 \\
b & 0 & 0 & 1 - a & b & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & b & 0 + a & 0 & 0 & b & 0 & 0 \\
0 & 0 & b & 0 & 0 & 0 - a & b & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & b & -1 + a & 0 & 0 & b & 0 \\
0 & 0 & 0 & 0 & b & 0 & 0 & -1 - a & b & 0 \\
0 & 0 & 0 & 0 & b & -2 + a & 0 & 0 & 0 & b \\
0 & 0 & 0 & 0 & b & 0 & 0 & 0 & -2 - a & 0 \\
\end{pmatrix}_{z}
\] (4.28)

where as in the $x$ basis, the Hamiltonian is
\[
\begin{pmatrix}
2 & -ia & b & 0 & 0 & 0 & 0 & 0 & 0 \\
-ia & 2 & 0 & -b & 0 & 0 & 0 & 0 & 0 \\
b & 0 & 1 & -ia & b & 0 & 0 & 0 & 0 \\
0 & -b & ia & 1 & 0 & -b & 0 & 0 & 0 \\
0 & 0 & b & 0 & 0 & -ia & b & 0 & 0 \\
0 & 0 & 0 & -b & ia & 0 & 0 & -b & 0 \\
0 & 0 & 0 & 0 & b & 0 & -1 & -ia & b \\
0 & 0 & 0 & 0 & 0 & b & 0 & -2 & -ia \\
0 & 0 & 0 & 0 & 0 & 0 & b & 0 & -1 \\
\end{pmatrix}
\]

where \(a = y/2\) and \(b = x/4\).

Additionally, in the \(n\bar{a}\) basis, I evaluate matrix elements for a Hamiltonian whose unperturbed part has been transformed and the perturbed part is the \(\omega_0 \sigma_z\) term

\[
H = n\omega - \frac{m^2 \eta^2}{4\omega} + \frac{\omega_0}{2} \sigma_z,
\]

so that the matrix elements will be calculated using Equation 4.12

\[
\frac{1}{\sqrt{2}} \left[ \langle + | \langle n'_+ | - im' (-| \langle n'_- | [n\omega + \frac{\omega_0 \sigma_z}{2}] \frac{1}{\sqrt{2}} [n_+]| +) + im|n_-| - \rangle \right].
\]

I have already shown the matrix elements of \(\sigma_z\) are

\[
\langle n', m' \sigma_z | n, m \rangle = \frac{1}{2} \left[ m J_q(x)(-1)^q + m' J_q(x) \right],
\]

and now the matrix elements for the constant \(n\omega\) are

\[
\frac{1}{\sqrt{2}} \left[ \langle + | \langle n'_+ | - im' (-| \langle n'_- | [n\omega] \frac{1}{\sqrt{2}} [n_+]| +) + im|n_-| - \rangle \right] = \frac{n\omega}{2} \delta_{n,n'}(1 + mm').
\]

Clearly, \(n\omega\)'s will lie along the diagonal as usual. A first few matrix elements are
\[ \langle +, 2 | n \omega + \frac{\omega_0 \sigma_z}{2} | 2, + \rangle = 2 \omega \frac{1}{2} \left[ \langle 2 | 2 \rangle + (1) \langle 2 | 2 \rangle \right] + \frac{\omega_0}{4} \left[ J_0(x)(-1)^{\theta} + J_0(x) \right] = 2 \omega + \frac{\omega_0 J_0(x)}{2} \]

\[ \langle +, 2 | n \omega + \frac{\omega_0 \sigma_z}{2} | 2, - \rangle = 0 \]

\[ \langle +, 2 | n \omega + \frac{\omega_0 \sigma_z}{2} | 1, + \rangle = 0 \]

\[ \langle +, 2 | n \omega + \frac{\omega_0 \sigma_z}{2} | 1, - \rangle = \omega \frac{1}{2} \left[ \langle 1 | 1 \rangle + (1) \langle 1 | 1 \rangle \right] + \frac{\omega_0}{4} \left[ J_1(x)(-1)^{\theta} - J_1(x) \right] = -\frac{\omega_0 J_1(x)}{2}, \]

so that the Hamiltonian after dividing by \( \omega \) up to \( n = 2 \) and \( J_2(x) \) is
\[
\begin{pmatrix}
2 + y J_0/2 & 0 & 0 & -y/2 J_1 & 0 \\
0 & 2 - y J_0/2 & -y/2 J_1 & 0 & y/2 J_2 \\
0 & y/2 J_1 & 1 + y J_0/2 & 0 & 0 \\
y/2 J_1 & 0 & 0 & 1 - y J_0/2 & -y/2 J_1 \\
0 & -y/2 J_2 & 0 & y/2 J_1 & 0 + y J_0/2 \\
y/2 J_2 & 0 & y/2 J_1 & 0 & 0 \\
0 & 0 & 0 & -y/2 J_2 & 0 \\
0 & 0 & y/2 J_2 & 0 & y/2 J_1 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & y/2 J_2 \\
\end{pmatrix}
\]

\[
\begin{pmatrix}
-y/2 J_2 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
-y/2 J_1 & 0 & -y/2 J_2 & 0 & 0 \\
0 & y/2 J_2 & 0 & 0 & 0 \\
0 & 0 & -y/2 J_1 & 0 & -y/2 J_2 \\
0 & 0 & 0 & -1 - y J_0/2 & -y/2 J_1 \\
y/2 J_1 & -1 + y J_0/2 & 0 & 0 & -y/2 J_1 \\
0 & 0 & -1 - y J_0/2 & -y/2 J_1 & 0 \\
-y/2 J_2 & 0 & y/2 J_1 & -2 + y J_0/2 & 0 \\
0 & y/2 J_1 & 0 & 0 & -2 + y J_0/2 \\
\end{pmatrix}
\]

where \( J_0 = J_0(x), J_1 = J_1(x), \) ... for the sake of compactness and I separated this large matrix into two, divided by columns 1-5 and 6-10. The arrows indicate that the full matrix should be joined by attaching the left side of the bottom matrix in Equation 4.35 with the right side of the top matrix.

I used the z basis for my computations. To diagonalize a Hamiltonian matrix by hand would be very tedious but using Matlab, I can easily use \( n = \pm 200 \) which will result in a matrix that is 802x802. I define \( N = 4 \times n + 1 \) so that \( N = 802 \) for that case. Such a huge matrix takes time to diagonalize but as \( N \) gets larger, the results become more and more accurate. For reference, an \( N = 802 \) computation takes about an hour to solve while an \( N = 1602 \) computation takes about 6.5 hours to solve.

### 4.4.2 Solving for Eigenvalues, Eigenvectors and Time Evolution Operators

Solving for the eigenvalues and eigenvectors will be the large majority of the computation. For calculating the expectation values of time dependent spin components, initialization of the state and spin matrices are needed. Specifically, in the z basis and an initial state \( \psi_0 \) along \(+x\), \( \psi_0 \) will take the form of a \( N \times 1 \) column vector of all ones (and normalized of course). The spin component operators will be \( N \times N \) matrices with 2x2 Pauli matrices along their respective diagonals.

I solve for the eigenvalues and eigenvectors by using a function I made that constructs the Hamiltonian matrix and then is given inputs in a separate script. The function that constructs the matrix
function myHamil = myBigHamiltonian(n, yB0, xBd)
% enters values of N, x and y into the hamiltonian
% yB0 = gamma3 * B0 / omegaDress
% xBd = gamma3 * Bd / omegaDress

a = yB0/2.0;
b = xBd/4.0;
N = n*4+2;
myHamil = zeros(N,N);

nrange = -n:n;
nrange = [nrange,nrange];
nrange = sort(nrange);
nrange = flip(nrange);

% diagonals
for i=1:length(nrange)
    myHamil(i,i) = nrange(i)+a*(-1)^(i+1);
end

% off diagonals
for i=1:length(nrange)
    if i == 1
        myHamil(i,i+3) = b;
    end
    if i == 2
        myHamil(i,i+1) = b;
    end
    if i > 2 && i < N-1
        if mod(i,2) == 0
            myHamil(i,i+1) = b;
            myHamil(i,i-3) = b;
        end
        if mod(i,2) == 1
            myHamil(i,i-1) = b;
        end
    end
end
\begin{verbatim}
myHamil(i,i+3) = b;
end
end
if i == N-1
    myHamil(i,i-1) = b;
end
if i == N
    myHamil(i,i-3) = b;
end
end

Such that the script that actually solves for the expectation values, includes the following commands

\begin{verbatim}
x = gamma3 * dressfield / dressfreq;
y = basefreq / dressfreq;
myHamil = myBigHamiltonian(n,y,x);
[eigenvec, eigenval] = eig(myHamil);
\end{verbatim}

With \( n \), \( \text{basefreq} \) and \( \text{dressfreq} \) specified at the beginning of the script. With the eigenvalues known, I move to calculating time evolution operators

\[
U_i = e^{-i w_i \lambda},
\] (4.36)

where \( t_i \) is just an element in the array \( t \) representing time and since I will use \( T = 10.0 \) s and \( \text{tstep} = 0.0005 \) s, \( t \) is a 1x20001 array. \( \lambda \) is the diagonal eigenvalues matrix so that \( U \) is an \( N \)x\( N \) diagonal matrix at a given time.

\( \psi(t) \) is constructed by transforming \( U \) into the eigenvector basis, letting it evolve, then transforming back and multiplying this onto \( \psi_0 \)

\[
\psi_i(t) = K^+ U_i(t) K \cdot \psi_0,
\] (4.37)

where \( K \) is the \( N \)x\( N \) eigenvector matrix. Finally, the expectation values over time take the usual form of

\[
S_i(t) = \psi(t)^+ S_i \psi(t).
\] (4.38)

The results are spin components as time arrays just like in the RK4 and I proceed to take fast Fourier transforms of them to extract frequencies. What I saw was agreement between this method and the RK4. At first, for low \( N \), the Hamiltonian method was all over the place. But as \( N \) got larger, the results converged towards what the RK4 showed. However, artifacts existed even for relatively high \( N \). You
will see in a couple tables that these artifacts decrease as $N$ increases. Whereas the expected and anomalous peaks increased for increasing $N$.

### 4.4.3 Comparing the Hamiltonian Method to the RK4

The Hamiltonian method showed reasonable results for $n = \pm 150$ which is $N = 602$. However, to be more accurate, I will use $n = \pm 200$ in the following plots. Figures 4.13 to 4.16 show $\sigma_y$ and $\sigma_z$ for $y = 0.10$ and $y = 0.01$ and as with the RK4 plots, I have zoomed in to show relevant frequencies.
Figure 4.15 $\sigma_z$ frequencies for $y=0.10$ using the Hamiltonian method, $N=802$.

Figure 4.14 $\sigma_x$ frequencies for $y=0.01$ using the Hamiltonian method, $N=802$. 
Figure 4.16 $\sigma_z$ frequencies for $y=0.01$ using the Hamiltonian method, $N=802$.

The immediate conclusion is that the Hamiltonian method is showing very similar results to the RK4 method. The difference in heights between the two methods mostly comes from the difference in time stepping and therefore total intensity. The ratio of heights between the two methods as well as the ratio of heights within a method and compared to the other would converge for $n$ much larger. And again, I am seeing the anomalous frequency heights decreasing as $y$ gets smaller. For comparison to Figures 4.10 to 4.12, I will loop through four values of $y$: 0.10, 0.05, 0.02 and 0.01 and show the results for $n = \pm 200$ in Figure 4.17. The reason I’m only using four values whereas the RK4 plots used 901 $y$ values is because each Hamiltonian method simulation takes time. What I will also do is use $n = \pm 150$ and collect all the frequencies where there’s a local maximum with height greater than 50. Then do the same for $n = \pm 250$. The results are shown in Tables 4.1-4.6.
Figure 4.17 $\sigma_y$ and $\sigma_z$ vs. frequency peaks solved for using the Hamiltonian method for $n = \pm 150$.

Table 4.1 $\sigma_y$ relevant frequency heights as $y$ changes and $n = \pm 150$

<table>
<thead>
<tr>
<th>y</th>
<th>$\omega_d$</th>
<th>Artifact</th>
<th>$\omega$</th>
<th>$\omega_d - 2\omega$</th>
<th>$\omega_d + 2\omega$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.10</td>
<td>9556.47</td>
<td>203.62</td>
<td>77.59</td>
<td>85.50</td>
<td>49.94</td>
</tr>
<tr>
<td>0.05</td>
<td>9772.16</td>
<td>131.84</td>
<td>22.03</td>
<td>26.81</td>
<td>28.54</td>
</tr>
<tr>
<td>0.02</td>
<td>9819.15</td>
<td>112.68</td>
<td>3.79</td>
<td>12.41</td>
<td>9.60</td>
</tr>
<tr>
<td>0.01</td>
<td>9825.37</td>
<td>110.00</td>
<td>0.79</td>
<td>7.34</td>
<td>7.54</td>
</tr>
</tbody>
</table>

Table 4.2 $\sigma_y$ relevant frequency heights as $y$ changes and $n = \pm 250$

<table>
<thead>
<tr>
<th>y</th>
<th>$\omega_d$</th>
<th>Artifact</th>
<th>$\omega$</th>
<th>$\omega_d - 2\omega$</th>
<th>$\omega_d + 2\omega$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.10</td>
<td>9600.16</td>
<td>191.50</td>
<td>78.16</td>
<td>86.28</td>
<td>50.30</td>
</tr>
<tr>
<td>0.05</td>
<td>9817.09</td>
<td>118.43</td>
<td>22.14</td>
<td>27.00</td>
<td>28.79</td>
</tr>
<tr>
<td>0.02</td>
<td>9864.37</td>
<td>98.40</td>
<td>3.80</td>
<td>12.52</td>
<td>9.67</td>
</tr>
<tr>
<td>0.01</td>
<td>9870.63</td>
<td>95.57</td>
<td>0.78</td>
<td>7.40</td>
<td>7.60</td>
</tr>
</tbody>
</table>
Table 4.3 $\sigma_y$ relevant frequency heights as $y$ changes and $n=\pm 150$

<table>
<thead>
<tr>
<th>$y$</th>
<th>$\omega_d$</th>
<th>Artifact</th>
<th>$\omega$</th>
<th>$\omega_d - 2\omega$</th>
<th>$\omega_d + 2\omega$</th>
<th>$3\omega$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.10</td>
<td>6470.37</td>
<td>157.79</td>
<td>802.08</td>
<td>1670.71</td>
<td>1002.44</td>
<td>63.96</td>
</tr>
<tr>
<td>0.05</td>
<td>6625.56</td>
<td>106.99</td>
<td>430.79</td>
<td>1043.54</td>
<td>1169.76</td>
<td>31.03</td>
</tr>
<tr>
<td>0.02</td>
<td>6658.52</td>
<td>92.14</td>
<td>182.74</td>
<td>1241.81</td>
<td>958.99</td>
<td>10.34</td>
</tr>
<tr>
<td>0.01</td>
<td>6662.85</td>
<td>90.03</td>
<td>70.60</td>
<td>1466.07</td>
<td>1506.60</td>
<td>5.25</td>
</tr>
</tbody>
</table>

Table 4.4 $\sigma_y$ relevant frequency heights as $y$ changes and $n=\pm 250$

<table>
<thead>
<tr>
<th>$y$</th>
<th>$\omega_d$</th>
<th>Artifact</th>
<th>$\omega$</th>
<th>$\omega_d - 2\omega$</th>
<th>$\omega_d + 2\omega$</th>
<th>$3\omega$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.10</td>
<td>6500.17</td>
<td>149.87</td>
<td>807.15</td>
<td>1685.39</td>
<td>1010.69</td>
<td>64.57</td>
</tr>
<tr>
<td>0.05</td>
<td>6656.19</td>
<td>97.12</td>
<td>433.77</td>
<td>1052.65</td>
<td>1179.41</td>
<td>31.32</td>
</tr>
<tr>
<td>0.02</td>
<td>6689.32</td>
<td>81.31</td>
<td>183.96</td>
<td>1251.65</td>
<td>966.64</td>
<td>10.44</td>
</tr>
<tr>
<td>0.01</td>
<td>6693.68</td>
<td>79.03</td>
<td>71.07</td>
<td>1478.99</td>
<td>1519.77</td>
<td>5.30</td>
</tr>
</tbody>
</table>

Table 4.5 $\sigma_z$ relevant frequency heights as $y$ changes and $n=\pm 150$

<table>
<thead>
<tr>
<th>$y$</th>
<th>$0\omega$</th>
<th>$\omega_d - \omega$</th>
<th>Artifact</th>
<th>$\omega_d + \omega$</th>
<th>$2\omega$</th>
<th>$\omega_d - 3\omega$</th>
<th>$\omega_d + 3\omega$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.10</td>
<td>1357.89</td>
<td>3520.33</td>
<td>28.90</td>
<td>4059.40</td>
<td>267.83</td>
<td>342.64</td>
<td>266.91</td>
</tr>
<tr>
<td>0.05</td>
<td>681.75</td>
<td>4736.81</td>
<td>34.29</td>
<td>3710.27</td>
<td>112.09</td>
<td>313.93</td>
<td>288.73</td>
</tr>
<tr>
<td>0.02</td>
<td>272.72</td>
<td>4778.47</td>
<td>30.18</td>
<td>4195.54</td>
<td>45.08</td>
<td>240.96</td>
<td>264.88</td>
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<tr>
<td>0.01</td>
<td>136.69</td>
<td>3860.59</td>
<td>26.46</td>
<td>3106.06</td>
<td>30.15</td>
<td>287.73</td>
<td>244.83</td>
</tr>
</tbody>
</table>

Table 4.6 $\sigma_z$ relevant frequency heights as $y$ changes and $n=\pm 250$

<table>
<thead>
<tr>
<th>$y$</th>
<th>$0\omega$</th>
<th>$\omega_d - \omega$</th>
<th>Artifact</th>
<th>$\omega_d + \omega$</th>
<th>$2\omega$</th>
<th>$\omega_d - 3\omega$</th>
<th>$\omega_d + 3\omega$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.10</td>
<td>1360.56</td>
<td>3541.45</td>
<td>26.59</td>
<td>4085.71</td>
<td>270.19</td>
<td>345.79</td>
<td>269.37</td>
</tr>
<tr>
<td>0.05</td>
<td>683.07</td>
<td>4769.78</td>
<td>26.87</td>
<td>3734.19</td>
<td>112.99</td>
<td>316.84</td>
<td>291.48</td>
</tr>
<tr>
<td>0.02</td>
<td>273.25</td>
<td>4810.54</td>
<td>20.14</td>
<td>4224.01</td>
<td>45.43</td>
<td>243.36</td>
<td>267.46</td>
</tr>
<tr>
<td>0.01</td>
<td>136.95</td>
<td>3886.70</td>
<td>17.13</td>
<td>3126.20</td>
<td>30.41</td>
<td>290.51</td>
<td>247.16</td>
</tr>
</tbody>
</table>

What's labeled above each column is the frequency the peak corresponds to - whether predicted by
theory (standard black text), an anomalous frequency (blue text) or an artifact (red text). The artifacts are peaks at frequencies that have no relevance and are only present because of numerical error. When artifact values in the tables are a line, my filter could not find them and I could not find them by manually searching. My filter of peaks greater than 50 was too stringent for \( \sigma_x \) anomalies and a few \( \sigma_y \) ones so I manually went to the plots and found them. As I suspected, values for artifacts decrease as \( N \) increases and those 'intensity' counts get redistributed to all other peaks including ones not predicted by theory. This is another confirmation that the Physics Report [Gol94] theory should be taken to higher order perturbation theory even if these peaks are small.

To bring everything full circle would be to take perturbation theory to higher order and show the new terms line up with what I’m seeing in these plots.

### 4.5 First Order Perturbation Theory, Corrections to the Eigenstates

#### 4.5.1 Spin Expectation Values up to First Order

In the first section, the degeneracy was lifted by finding first order energy shifts. The \( m_z \) eigenvectors were then used for calculating expectation values. Given the evidence laid out in the sections showing results from the RK4 and Hamiltonian methods, it’s clear extensions of perturbation theory are needed to account for the anomalous frequencies. More specifically, corrections to the eigenstates are required rather than corrections to the eigenvalues. This is because the only way for the peak heights to have a dependence on \( y^n \), where \( n \) is the order of perturbation theory, is from corrections to the eigenstates. Whereas corrections to the eigenvalues introduce changes to energy levels and therefore frequencies dependent on \( y \) and corrections to the critical dressing condition.

An expansion of an eigenstate using perturbation theory corrections goes as

\[
|n, m\rangle = |n, m\rangle^{(0)} + |n, m\rangle^{(1)} + ... \tag{4.39}
\]

The second term is the 1st order correction whereas the first term are the \( m_z \) eigenstates

\[
|n, m\rangle = \frac{1}{\sqrt{2}} \left[ |n_+\rangle |+\rangle + im |n_-\rangle |-\rangle \right]. \tag{4.40}
\]

The first order correction is generally written as

\[
|n^{(1)}\rangle = \sum_{k \neq n} \frac{\langle k |V|n\rangle^{(0)}}{E_n^{(0)} - E_k^{(0)}} |k\rangle^{(0)}, \tag{4.41}
\]

so that I can construct first order corrections to unprimed and primed states:
where I define $A$ as

$$A(m, m', q') = \frac{m J_q(x)(-1)^{q'} + m'' J_q'(x)}{4 q'}.$$  \hspace{1cm} (4.43)

For the primed states

$$|n', m'\rangle^{(1)} = \sum_{n'', m''} \frac{1}{\sqrt{2}} \omega_0 \sigma_x |n', m'\rangle |n'', m''\rangle$$

$$= \sum_{m'} \sum_{q' \neq 0} \frac{1}{\sqrt{2}} \omega_0 \sigma_x |m' J_q(x)(-1)^{q'} + m'' J_q'(x)|n', m'\rangle |n'', m''\rangle$$  \hspace{1cm} (4.44)

$$= y \sum_{m'} \sum_{q' \neq 0} A'(m, m', q', q') |n'', m''\rangle,$$

where I define $A'$ as

$$A'(m, m', q, q') = \frac{m' J_q(x)(-1)^{(q'-q)} + m'' J_q'(x)}{4 (q' - q)}.$$  \hspace{1cm} (4.45)

From before, $q = n - n'$ but now $q' = n - n''$ such that $n' - n'' = q' - q$. And because states can't be equal in the formulation of first order corrections to eigenstates, $q' \neq 0$ and $q' - q \neq 0$.

Now a state $|n, m\rangle$ up to first order is

$$|n, m\rangle = \frac{1}{\sqrt{2}} \left[ |n_+\rangle + i m |n_-\rangle \right] + y \sum_{n'', m''} \sum_{q' \neq 0} A(m, m', q') \left[ |n''_+\rangle + i m'' |n''_-\rangle \right].$$  \hspace{1cm} (4.46)

And a state $|n', m'\rangle$ up to first order is similarly

$$|n', m'\rangle = \frac{1}{\sqrt{2}} \left[ |n'_+\rangle + i m' |n'_-\rangle \right] + y \sum_{n'', m''} \sum_{q' \neq 0} A'(m, m', q, q') \left[ |n'''_+\rangle + i m'' |n'''_-\rangle \right].$$  \hspace{1cm} (4.47)
The matrix elements for $\sigma_y$ are

$$
\langle n', m'| \sigma_y | n, m \rangle 
= \frac{1}{2} \left[ \langle +| \langle n'_+| - im' \langle -| \langle n'_-| \rangle + yA^*(m, m', q, q') \langle +| \langle n''_+| - im'' \langle -| \langle n''_-| \rangle \right] 
\times \left[ |+\rangle \langle -| + |\rangle \langle +| \right] 
\times \left[ \langle n'_+| + im|n'_-| \rangle + yA(m, m', q') \langle n''_+| + im''|n''_-| \rangle \right] 
\times \left[ |n'_+| + im|n'_-| \rangle + yA(m, m', q') \langle n''_+| + im''|n''_-| \rangle \right]
$$

(4.48)

$$
\langle n', m'| \sigma_y | n, m \rangle 
= \frac{1}{2} \left[ im\langle n'_+| n_- \rangle - im\langle n'_-| n_+ \rangle 
+ yA^*(m, m', q, q') im\langle n''_+| n_- \rangle - yA^*(m, m', q, q') im\langle n''_-| n_+ \rangle 
- yA(m, m', q') im\langle n''_-| n'_+ \rangle + yA(m, m', q') im\langle n''_+| n'_- \rangle + O(y^2) \right].
$$

where the first two terms in the brackets are the usual zeroth order, unperturbed terms and $O(y^2)$ refers to terms proportional to $y^2$ that I will ignore.

Then, the expectation value is

$$
< \sigma_y(t)> = \sum_{m, m', q, q'} \sum_{m, m', q, q'} \frac{1}{2} a_n^* a_n e^{iq\omega t} e^{i(m-m')\omega_d t/2} \left[ imJ_q(x)(-1)^q - im' J_q(x) \right] 
+ iy \left[ m' J_{q'-q}(x)(-1)^{q'-q} + m'' J_{q'-q}(x) \right] \frac{4(q'-q)}{4(q'-q)} \left[ mJ_q'(x)(-1)^q - m'' J_q(x) \right] 
+ iy \left[ mJ_q'(x)(-1)^q + m'' J_{q'-q}(x) \right] \frac{4q'}{4q'} \left[ -m' J_{q'-q}(x) + m'' J_{q'-q}(x)(-1)^q \right].
$$

(4.49)

Next I will choose $m = m'$ so that $\omega_d$ no longer contributes to any frequency. Then, I examine the four cases when $m, m' = \pm 1$ and $m'' = \pm 1$. These calculation are located in the appendix in A3. I know from the RK4 and diagonalizing the Hamiltonian that for $\sigma_y$, the anomalous peaks are for odd $q$. Choosing odd $q$, then varying $q'$ (which dictates whether $q' - q$ is even or odd), I have
where the expression after the arrow can use whichever value of \( q \). For the terms in the large braces \( q \) equal but opposite sign for certain \( q \) and \( q' \) even, \( q' \) odd, \( q \) odd \( q' \) even, \( q' \) odd, \( q = 1 \) and I choose different values of \( q' \) based off the sum rules. For the terms in the large braces

\[
\begin{aligned}
\sum_{q \geq 0, \text{odd}} & \frac{1}{2} [e^{iq\omega t} + e^{-iq\omega t}] iy \\
\times \left\{ \sum_{q' \text{ odd}, q' \sim q \text{ even}} \left[ \frac{J_q(x)J_{q'-q}(x) + J_{q'}(x)J_{q'-q}(x)}{q'} + \frac{-J_{q'-q}(x)J_q(x) - J_{q'-q}(x)J_q(x)}{q' - q} \right] \\
+ \sum_{q' \text{ even}, q' \sim q \text{ odd}} \left[ \frac{-J_{q'-q}(x)J_q(x) - J_{q'}(x)J_{q'-q}(x)}{q'} + \frac{-J_{q'-q}(x)J_q(x) - J_{q'-q}(x)J_q(x)}{q' - q} \right] \right\} \\
= & \ i y \sum_{q \geq 0, \text{odd}} \cos q \omega t \\
\times \left\{ \sum_{q' \text{ odd}, q' \sim q \text{ even}} \left[ \frac{J_q(x)J_{q'-q}(x) + J_{q'}(x)J_{q'-q}(x)}{q'} + \frac{-J_{q'-q}(x)J_q(x) - J_{q'-q}(x)J_q(x)}{q' - q} \right] \\
+ \sum_{q' \text{ even}, q' \sim q \text{ odd}} \left[ \frac{-J_{q'-q}(x)J_q(x) - J_{q'}(x)J_{q'-q}(x)}{q'} + \frac{-J_{q'-q}(x)J_q(x) - J_{q'-q}(x)J_q(x)}{q' - q} \right] \right\},
\end{aligned}
\]

(4.50)

with \( J_q(x) \) and \( J_{q'-q}(x) \) commuting. Of the four terms in Equation 4.50, the first and the fourth will be equal but opposite sign for certain \( q \) and \( q' \) values. Whereas the second and the third will be equal and same sign. I will show two examples of this when \( q = 1 \) and I choose different values of \( q' \) based off the sum rules. For the terms in the large braces

First sum choose \( q' = -1 \), Second sum choose \( q' = 2 \)

\[
\begin{aligned}
\left\{ \frac{-J_1(x)J_2(x) - J_1(x)J_2(x)}{(-1)} + \frac{J_2(x)J_1(x) + J_2(x)J_1(x)}{(-2)} \\
+ \frac{-J_2(x)J_1(x) - J_2(x)J_1(x)}{(2)} + \frac{-J_1(x)J_2(x) - J_1(x)J_2(x)}{(1)} \right\} \\
= & \ \frac{-4J_1(x)J_2(x)}{2} \rightarrow \frac{-4J_{q'-q}(x)J_q(x)}{q'},
\end{aligned}
\]

(4.51)

where the expression after the arrow can use whichever value of \( q' \). For the next closest choices
First sum choose \( q' = 3 \), Second sum choose \( q' = -2 \)

\[
\begin{align*}
\left\{ \frac{J_3(x)J_2(x) + J_3(x)J_2(x)}{3} \right. & - \frac{J_2(x)J_3(x) - J_2(x)J_3(x)}{2} \right. \\
& + \left. \frac{-J_2(x)(-1)J_3(x) - J_2(x)(-1)J_3(x)}{(-2)} \right. \\
& + \left. \frac{-(-1)J_3(x)J_2(x) - (-1)J_3(x)J_2(x)}{(-3)} \right. \\
= & \frac{-4J_2(x)J_3(x)}{2} \rightarrow \frac{-4J_{q'-q}(x)J_q(x)}{q'}.
\end{align*}
\]

(4.52)

So that finally, Equation 4.49 can be written as

\[
\langle \sigma_y(t) \rangle |_{m=m'} = -4i y \sum_{q>0, odd \, q' \neq 0, \, even} \sum \cos q \omega t \frac{J_{q'-q}(x)J_q(x)}{q'},
\]

(4.53)

for \( m = m' \) and odd \( q \). The first few terms are

\[
-4i y \left[ \cos \omega t \left( \frac{J_1(x)J_2(x)}{2} \right) + \cos \omega t \left( \frac{J_3(x)J_2(x)}{2} \right) + \cos 3 \omega t \left( \frac{J_1(x)J_2(x)}{2} \right) + \cos 3 \omega t \left( \frac{J_5(x)J_2(x)}{2} \right) + \ldots \right]
\]

(4.54)

\[
= -2i y J_2(x) \left[ J_1(x) + J_3(x) \right] \cos \omega t + \left[ J_5(x) - J_1(x) \right] \cos 3 \omega t + \ldots.
\]

For all the other cases \( (m \neq m' \) with \( q \) odd or even and \( m = m' \) with even \( q \) \) all terms vanish. I show examples of this in Appendix A3.

For \( \sigma_z \), the matrix elements are

\[
\langle n', m' | \sigma_z | n, m \rangle
= \frac{1}{2} \left[ \left[ \langle n'_+ | + i m' (-|n'_-| - i m'' (-|n''_-|) \rangle + y A^* \langle n'_+ | + i m'' (-|n''_-|) \rangle \right.ight.
\]

\[
\left. \times \left[ (-i |+) + i (-|-) \left\langle \right. + \right. \right.
\]

\[
\left. \times \left[ \langle n_+ | + i m |n_-| \rangle \left. + \right. \right. \right.
\]

\[
\left. \times \left( y A \langle n''_+ | + i m'' |n''_-| \rangle \right) \right] \right] \right] + y A^* m \langle n'_+ | n''_- | n_+ \rangle + y A^* m'' \langle n'_+ | n''_- | n_+ \rangle
= \frac{1}{2} \left[ m J_q(x)(-1)^q + m' J_q(x)
\]

\[
+ m y A^* J_{q'}(x)(-1)^q + m'' y A^* J_{q'}(x) + m' y A J_{q'-q}(x) + m'' y A J_{q'-q}(x)(-1)^{q'-q} + O(y^2) \right] \right]
\]

(4.55)

So that the expectation value up to \( y \) is
with the first 4 terms being Appendix A4. Then the linear in y terms are

This time, I’ll exclude the zeroth order terms. The calculation for the sum over spins for \( m = m' \) is in Appendix A4. Then the linear in y terms are

\[
<\sigma_z(t)> = \sum_{m,m',m''} \sum_{q,q',q''} \frac{1}{2} a_n^* a_n e^{i\omega t} e^{i(m-m')\omega_d t/2} \left[ m J_q(x)(-1)^q + m' J_q(x) + m'' y A J_{q'-q}(x) + m' y A J_{q''}(x)(-1)^{q'-q} \right].
\] (4.56)

and remembering that for \( \sigma_z(t) \), I saw the anomalies are for even \( q \). Then I have

\[
<\sigma_z(t)> = \sum_{q \geq 0, even} \frac{1}{2} \left[ e^{i\omega t} + e^{-i\omega t} \right] y 
\times \left\{ \sum_{q', odd, q'' - q' odd} \frac{J_{q' - q}(x) J_q(x) + J_{q'' - q}(x) J_{q'}(x)}{q' - q} + \frac{-J_q(x) J_{q' - q}(x) - J_{q''}(x) J_{q'}(x)}{q'} \right\} + \sum_{q' even, q'' - q even} \frac{J_{q' - q}(x) J_q(x) + J_{q'' - q}(x) J_{q'}(x)}{q' - q} + \frac{J_q(x) J_{q' - q}(x) + J_{q''}(x) J_{q'}(x)}{q'} \right\}
\] (4.57)

with the first 4 terms being

\[
<\sigma_z(t)> = 4y \left[ J_1(x) J_1(x) + J_{-1}(x) J_{-1}(x) \right] (2) - \cos 2\omega t \left[ J_1(x) J_1(x) \right] (1) - \cos 2\omega t \left[ J_0(x) J_0(x) \right] (1) \right]
\] (4.58)

For \( \sigma_x \), I saw anomalous frequencies at \( q \omega \) and \( \omega_d \pm 2\omega \). The matrix elements for \( \sigma_x \) are

\[
\left( \text{For } \sigma_x, \text{ I saw anomalous frequencies at } q \omega \text{ and } \omega_d \pm 2\omega \right)
\]
\[ \langle n', m' | \sigma_x | n, m \rangle \]
\[ = \frac{1}{2} \left[ \langle + | \langle n' | - i m' \langle - | n' \rangle | + A^* \langle + | \langle n'' | - i m'' \langle - | n'' \rangle | + \left[ \langle n_+ | + \rangle + i m n_+ \langle - | \right] + A \langle n''_+ | + \rangle + i m'' \langle n''_+ | - \rangle \right] \times \left[ \langle n_+ | + \rangle + i m n_+ \langle - | \right] + A \langle n''_+ | + \rangle + i m'' \langle n''_+ | - \rangle \right] \]
\[ = \frac{1}{2} \left[ \langle + | \langle n' | - i m' \langle - | n' \rangle + A^* \langle + | \langle n'' | - i m'' \langle - | n'' \rangle \right] \times \left[ \langle n_+ | + \rangle + i m n_+ \langle - | \right] + A \langle n''_+ | + \rangle + i m'' \langle n''_+ | - \rangle \right] \]
\[ = \frac{1}{2} \left[ \langle n' | n_+ \rangle - m m' \langle n'_+ | n_+ \rangle + A \langle n'' | n_+ \rangle - m m'' \langle n''_+ | n_+ \rangle \right] + A \langle n' | n_+ \rangle - m m' \langle n'_+ | n_+ \rangle + O(y^2) \]
\[ = \frac{1}{2} \left[ (1 - m m') \delta_{n,n'} + A(1 - m m'') \delta_{n,n''} + A(1 - m' m'') \delta_{n',n''} \right]. \]  

(4.60)

so that the expectation value is

\[ < \sigma_x(t) > = \sum_{m,n,m'} \sum_{n',n''} \frac{1}{2} a_n^* e^{i q \omega t} e^{i (m-m') \omega dt} \left[ (1 - m m') \delta_{n,n'} \right. \]
\[ + A(1 - m m'') \delta_{n,n''} + A(1 - m' m'') \delta_{n',n''}. \]  

(4.61)

For summing over all \( n \)’s and \( m \)’s in Equation 4.61, I have the following cases and their constraints (due to \( k \neq n \) in the formulation for first order perturbation theory)

\[ n = n', \quad n'' \neq n \rightarrow n'' \neq n' \rightarrow \text{no m constraints}; \]
\[ n = n', \quad n'' = n \rightarrow n'' = n' \rightarrow m'' \neq m', \quad m'' \neq m; \]
\[ n \neq n', \quad n'' \neq n \rightarrow n'' = n' \rightarrow m'' \neq m'; \]
\[ n \neq n', \quad n'' = n \rightarrow n'' \neq n' \rightarrow m'' \neq m. \]

(4.62)

Of these four cases, the first leads to the zeroth order \( \cos \omega_d t \) term. The second case has \( q' = 0 \) and \( q' - q = 0 \) which is not allowed. Cases three and four are the ones I care about. Given I’m in a spin 1/2 system, a constraint like \( m'' \neq m' \) means \( m'' = -m \) and so I can simply replace all \( m'' \)’s by \(-m\). Also, the third case has \( q' - q = 0 \) so that any \( q' \) can be replaced by \( q \). And the fourth case has \( q' = 0 \) but given \( n'' \neq n' \), there’s no singularity.

The calculation for the third case is
\[
\sum_{m',m''} \sum_{n,n'} \frac{1}{2} a^*_n a_m e^{i \theta_m} e^{i(m-m') \omega_d t/2} y \frac{m J_q(x)[(-1)^q + m'' J_{q'}(x)]}{4} [1-m'' m'']
= \sum_{q} \sum_{m',m''} \frac{1}{2} e^{i \theta_m} e^{i(m-m') \omega_d t/2} y \frac{m' J_{q'-q}(x)[(-1)^q - m' J_{q'}(x)]}{4q}
\]
\[
= y \sum_{q} e^{i \theta_m} \frac{J_q(x)}{4q} \left[ (-1)^q - 1 \right] + e^{-i \theta_m} \left[ (-1)^q + 1 \right] + e^{i \theta_m} \left[ (-1)^q + 1 \right] + \left[ (-1)^q - 1 \right]
\]
(4.63)
\[
= y \sum_{q>0, \text{even}} e^{i \theta_m} \frac{J_q(x)}{4q} \left( 2(2i \sin \omega_d t) \right)
\]
\[
= 2i y \sum_{q>0, \text{even}} \frac{J_q(x)}{q} \cos q \omega t \sin \omega_d t.
\]

And the fourth case
\[
\sum_{m',m''} \sum_{n,n'} \frac{1}{2} a^*_n a_m e^{i \theta_m} e^{i(m-m') \omega_d t/2} y \frac{m' J_{q'-q}(x)[(-1)^q - m'' J_{q'}(x)]}{4} [1-m'' m'']
= \sum_{q} \sum_{m',m''} \frac{1}{2} e^{i \theta_m} e^{i(m-m') \omega_d t/2} y \frac{m' J_{q'-q}(x)[(-1)^q - m'' J_{q'}(x)]}{4} [1+ m'^2]
\]
\[
= -y \sum_{q} \sum_{m,m'} e^{i \theta_m} e^{i(m-m') \omega_d t/2} \frac{m' J_{q'-q}(x) - m J_{q'}(x)[(-1)^q]}{2q}
\]
\[
= -\frac{1}{2} y \sum_{q} e^{i \theta_m} \frac{J_q(x)}{2q} \left[ 1 - (-1)^q \right] + e^{-i \theta_m} \left[ 1 + (-1)^q \right] + e^{i \theta_m} \left[ -1 + (-1)^q \right] + \left[ -1 + (-1)^q \right]
\]
(4.64)
\[
= -y \sum_{q} e^{i \theta_m} \frac{J_q(x)}{4q} \left[ 1 + (-1)^q \right] \left[ e^{-i \theta_m} - e^{i \theta_m} \right]
\]
\[
= -y \sum_{q>0, \text{even}} e^{i \theta_m} \frac{J_q(x)}{4q} \left( 2(-2i \sin \omega_d t) \right)
\]
\[
= 2i y \sum_{q>0, \text{even}} \frac{J_q(x)}{q} \cos q \omega t \sin \omega_d t.
\]

Adding together the results from the third and fourth cases gives the full linear in y dependence of \( \sigma_x \) as
\[
4i y \sum_{q>0, \text{even}} \frac{J_q(x)}{q} \cos q \omega t \sin \omega_d t.
\]
(4.65)

From the results of Equation 4.65, it can be seen that the \( \sigma_x \omega_d \pm q \omega \) for even \( q \) anomaly has been resolved. Also just as important is that the \( q \omega \) anomaly did not show itself since data in the earlier
section suggested it would depend on \(y^2\). The \(y^2\) terms from the first order corrections that I ignored plus the \(y^2\) terms that would come about in second order corrections should show the frequencies \(q \omega\) for odd \(q\).

Incorporating the first few terms into the theoretical expression in the RK4 looks like

\[
\begin{align*}
Sx\_theory(s,:) &= \cos(\omega_d t) \\
&+ 4*1i*y*besselj(2,x\_eff)/2.*\cos(2*\omega*t).*\sin(\omega_d t); \\
Sy\_theory(s,:) &= -besselj(0,x\_eff)*\sin(\omega_d t) \\
&- besselj(2,x\_eff)*(\sin((2*\omega+\omega_d)*t)+\sin((-2*\omega+\omega_d)*t)) \\
&- besselj(4,x\_eff)*(\sin((4*\omega+\omega_d)*t)+\sin((-4*\omega+\omega_d)*t)) \\
&- 2*1i*y*besselj(2,x\_eff)*((besselj(1,x\_eff)+besselj(3,x\_eff))*\cos(\omega*t) \\
&+ (besselj(5,x\_eff)-besselj(1,x\_eff))*\cos(3*\omega*t)); \\
Sz\_theory(s,:) &= besselj(1,x\_eff)*(\cos((1*\omega-\omega_d)*t)-\cos((1*\omega+\omega_d)*t)) \\
&+ besselj(3,x\_eff)*(\cos((3*\omega-\omega_d)*t)+\cos((3*\omega+\omega_d)*t)) \\
&+ 4*y*(.05-\cos(2*\omega*t)*besselj(1,x\_eff)*(besselj(1,x\_eff)-besselj(3,x\_eff))); \\
Sx\_theory\_fftshift(s,:) &= fftshift(abs(fft(Sx\_theory(s,:)))); \\
Sy\_theory\_fftshift(s,:) &= fftshift(abs(fft(Sy\_theory(s,:)))); \\
Sz\_theory\_fftshift(s,:) &= fftshift(abs(fft(Sz\_theory(s,:))));
\end{align*}
\]

The plots with the first order corrections added to the theory, analogous to Figures 4.5-4.7 are shown below in Figures 4.18-4.20.
Figure 4.18 $\sigma_x$ for $y = 0.10$, frequencies solved for using the RK4 method. The $\omega \pm 2\omega$ frequencies are now accounted for with the first order corrections to the eigenstates. The bottom plot shows the anomalies with a zoomed-in view.
Figure 4.19 $\sigma_y$ for $y = 0.10$, frequencies solved for using the RK4 method. The $\omega$ and $3\omega$ frequencies are now accounted for with the first order corrections to the eigenstates. The bottom plot shows the anomalies with a zoomed-in view.
Figure 4.20 $\sigma_y$ for $y = 0.10$, frequencies solved for using the RK4 method. The $0\omega$ and $2\omega$ frequencies are now accounted for with the first order corrections to the eigenstates. The bottom plot shows the anomalies with a zoomed-in view.

The theory for the anomalies is included in Figures 4.18-4.20. Of course, there are more not shown that are very small that I would need to put more terms into Matlab to account for them. In Figure 4.18, the $\omega_d\pm2\omega$ theoretical heights in black from the first order corrections are too large. In Figure 4.19,
the $\omega$ theory peak is too small while the $3\omega$ is too large. Figure 4.20 has discrepancies between RK4 heights and the new terms added to the theory as well. I also simply used 0.10 as a placeholder for the $q = 0$ oscillatory term. The differences are most likely due to either factors of 2 missing for certain frequency amplitudes, missing Bessel function terms since I stopped the sums after two terms or issues with normalization for Fourier transforms in Matlab.
5.1 Theory

5.1.1 Motivation

The nEDM experiment relies on UCN-\(^3\)He absorption which means their mutual interaction is of utmost importance. There will be a \(^3\)He pseudomagnetic field present that only the neutrons will feel. Modulation of the dressing field will be used to offset this field. The scattering length for the neutron-\(^3\)He interaction is complex and can be decomposed into coherent and incoherent components. The scattering length is spin dependent and this is exploited in the nEDM experiment. The imaginary terms control the absorption rate and lead to the near zero cross section when the spins are parallel and large cross section when the spins are antiparallel. Whereas, the real terms give the Abragam pseudomagnetic field - the Fermi potential is spin dependent and mimics a magnetic field potential. As measured by Koester et al. [Koe], the coherent and incoherent scattering lengths are

\[
b_c = 5.73 - 1.483i \text{ fm and } b_i = -2.5 + 2.568i \text{ fm},
\]

(5.1)

giving

\[
b_+ = b_c + \sqrt{\frac{I}{I+1}} b_i = 4.29 + 0i \text{ fm}
\]

\[
b_- = b_c - \sqrt{\frac{I}{I+1}} b_i = 10.07 - 5.93i \text{ fm};
\]

(5.2)
where + and − refer to spins parallel and antiparallel respectively and \( I \) is nuclear spin. For neutrons and \(^3\)He in the x-y plane, neutrons will precess about the helium spins and on average, the pseudomagnetic field will remain in the x-y plane. This means the pseudomagnetic field is perpendicular to the electric field and reduces nEDM sensitivity.

Given the pseudomagnetic field is only seen by the neutrons, a deviation away from critical dressing is created as an extra field term will push the neutron effective Larmor frequency away from \(^3\)He Larmor frequency. And although the pseudomagnetic field is quite small, about \( 1 \cdot 10^{-11} \)T for the experiment’s \(^3\)He concentrations of \( x = 10^{-10} \) and near perfect polarization, it must be accounted for because of the high precision of the nEDM experiment. The pseudomagnetic field will be parallel to the \(^3\)He spins and will have some average field value. In the lab frame on critical dressing, there were UCN and \(^3\)He precessing about the z-axis while undergoing an oscillating precession about the x-axis. UCN will have a small additional precession about the \(^3\)He and pick up a relative phase shift. Qualitatively, there would be separation that grows in time between the blue and red curves in Figure 4.4. The goal then is to offset this phase shift with dressing field modulations. The modulations will put the UCN and \(^3\)He in front or behind one another and create a symmetry about critical dressing that offsets the asymmetric phase shift from the pseudomagnetic field. The following section will derive the theory for modulations and underscore the lack of dependence \( <\sigma_x(t)> \) has on the pseudomagnetic field strength.

### 5.1.2 The Hamiltonian and Effect on Expectation Values

To start, the type of modulations I will use are square wave pulses and as stated, the idea is to alternate the relative positions of the UCN and \(^3\)He. For the dressing field, either \( \omega \) or \( \omega_1 \) can be modulated. I chose the latter because the former would be hard to implement in an experiment and changes the value of \( y = \omega_0/\omega \) when the perturbation strength should remain constant for a given simulation. What the modulation of \( \omega_1 \) means for my simulations is I will alternate between an effective \( x_1 \) and \( x_2 \) and hence \( B_{rf1} \) and \( B_{rf2} \) where \( B_{rf} \) was defined in Equation 4.23.

\[
B_{rf1} = (x_c + x_m)\omega/\gamma_n \\
B_{rf2} = (x_c - x_m)\omega/\gamma_n,
\]

(5.3)

where \( x_m \) is the square wave modulation. In this chapter, I will use \( B_{rf} \) instead of \( B_1 \) since there will be two different amplitudes with modulation on. Then modulating about \( x_c \) gives a relative precession frequency \( \omega_z \) between UCN and \(^3\)He

\[
\omega_{z+} = -\gamma B_0[J_0(x_c \pm x) - \alpha J_0(\alpha(x_c \pm x))] \\
\omega_{z1} = -\gamma B_0[J_0(x_c + x_m) - \alpha J_0(\alpha(x_c + x_m))] \\
\omega_{z2} = -\gamma B_0[J_0(x_c - x_m) - \alpha J_0(\alpha(x_c - x_m))] \\
\omega_{z1} = -\omega_{z2}
\]

(5.4)

There is an important assumption in Equation 5.4: a modulation of \( +x_m \) vs \( -x_m \) will lead to a UCN-\(^3\)He relative frequency of equal magnitude but opposite sign. I will show in the next section that this
assumption is wrong for the field parameters the nEDM experiment will use.

The modulation needs to be symmetric about $x_c$ so the square wave pulses will be applied for a
time $\tau/2$ with $+x_m$ then $\tau$ with $-x_m$ then $\tau$ with $+x_m$ and so on until the simulation ends. The relative
spin angle will have amplitude $\phi = \pm \omega_z \tau/2$. Starting with the following Hamiltonian, I will derive the
effect of square wave modulation as done in [Gol94]. The Hamiltonian is

$$H_\pm = -\frac{1}{2} \left[ \frac{1}{\tau_0} - \frac{P_3}{\tau_3} \right] \mathbf{\sigma}_n \cdot \mathbf{\sigma}_3 \pm \omega_z \mathbf{\sigma}_z \cdot \hat{z}$$

$$= -\frac{1}{2} \left[ \frac{1}{\tau_{w,\beta}} + \frac{1}{\tau_3} \right] \left( 1 - P_3 \mathbf{\sigma}_n \cdot \mathbf{\sigma}_3 \right) + AP_3 \mathbf{\sigma}_n \cdot \mathbf{\sigma}_3 \pm \omega_z \mathbf{\sigma}_z \cdot \hat{z}$$

$$= -\frac{i}{2\tau_0} \left[ \frac{1}{\tau_{w,\beta}} + \frac{1}{\tau_3} \right] + AP_3 \mathbf{\sigma}_n \cdot \mathbf{\sigma}_3 \pm \omega_z \mathbf{\sigma}_z \cdot \hat{z},$$

and for a classical field $\mathbf{\sigma}_3$ along the $x$ direction, the Hamiltonian in matrix form is

$$H_\pm = -\frac{i}{2\tau_0} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} \pm \omega_z & P_3 A' \\ P_3 A' & \mp \omega_z \end{pmatrix}.$$  (5.6)

$1/\tau_0 = 1/\tau_{w,\beta} + 1/\tau_{He}$ is a time scale for neutron losses via wall absorption, beta decay and helium
absorption. $A$ is the strength of the pseudomagnetic field, $A' = A + i/2\tau_3$ and $P_3$ is a measurement of the
$^3$He polarization which will be assumed to be equal to 1 in my simulations. The rest of the derivation
can be found in Appendix A6 with the result being the expectation value of $\sigma_x$ is independent of the
pseudomagnetic field strength $A$ due to the modulation

$$<\sigma_x(t)>=\pm \frac{1}{4} e^{-T/\tau_0} e^{\pm 2P_3 T/\tau_3 \sin \omega_z \tau} \cos \omega_z \tau. \quad (5.7)$$

The next question is whether $(+x_m, -x_m)$ leads to $(\omega_{z1}, \omega_{z2})$ where $\omega_{z1} = -\omega_{z2}$. The next section
addresses this and starts with the structure of the zeroth order Bessel function of the first kind.

### 5.2 A Question of Symmetric or Asymmetric Modulation

#### 5.2.1 The Zeroth Order Bessel Function Structure

The zeroth order Bessel function of the first kind looks roughly like a decaying sinusoidal curve. Bessel
functions are solutions to Bessel’s differential equation

$$x^2 \frac{d^2 y}{dx^2} + x \frac{dy}{dx} + (x^2 - a^2)y = 0. \quad (5.8)$$

$J_0(x)$, the solution to Equation 5.8, can be expanded around $x = 0$ (which was the form used in [Pol65])
and be expressed as

$$J_0(x) = \sum_{m=0}^{\infty} \frac{(-1)^m}{m! \Gamma(m + a + 1)} \left( \frac{x}{2} \right)^{2m+a}.$$  (5.9)
The plot of \( J_0(x) \) is shown in Figure 5.1. As previously mentioned, critical dressing is defined when the Larmor precession frequencies between UCN and \(^3\)He are equal effectively meaning \( \gamma'_n = \gamma'_3 \). The condition for critical spin dressing for UCN and \(^3\)He in a static magnetic field \( B_0 \) and oscillating dressing field \( B_x = B_{rf} \cos \omega t \) is

\[
-\gamma_n B_0 [J_0(x_c) - \alpha J_0(\alpha x_c)] = 0, \tag{5.10}
\]

where \( x_c = \omega_1 / \omega \), \( \omega_1 = -\gamma B_{rf} \) and \( \alpha = 1.112081855 \) is the ratio \( \gamma_3 / \gamma_n \). The solution is \( x_c = 1.1890180 \). However, a caveat is that Equation 5.10 is a condition for critical dressing in the limit \( Y = \omega / \omega_0 \gg 1 \).

For instance, from the Swank, Liu and Filippone paper [CS18], for \( Y = 9.81 \) (the nEDM experiment will use \( Y = 10 \)), the simulated critical dressing parameter will differ from the analytical one by about \(-0.466\%\). My simulations have near agreement with the values from that paper.

**Figure 5.1** The zeroth order Bessel function of the first kind.

When the dressing field is set for critical dressing, the neutrons and Helium precess about the z-axis at the same rate. Since dressing is controlling the relative rate, a change in \( x \) has the effect, when averaged over, of producing a \( \delta \omega \) about the z-axis between the UCN and \(^3\)He as shown in Equation 5.4. What I will show is that due to the derivatives of the zeroth order Bessel function, symmetric modulation will not nullify pseudomagnetic field effects. Not only will asymmetric modulation be needed, but there needs to be higher order corrections to Equations 5.4. Figure 5.2 shows the plot of the absolute value of the Bessel function terms in the brackets of Equation 5.10.
Figure 5.2 The absolute value of the critical dressing condition where the y-axis is the relative frequency between UCN and $^3\text{He}$, $\omega_z$, divided by $\omega_0$.

The first zero is at the critical dressing point the experiment and my simulations will use because the nEDM term gets diluted by the Bessel function correction so the largest value of $J_0(x)$ should be used. By inspection, the difference in y values, $(\omega_{z1} - \omega_{z2})/\omega_0$ where $\omega_0$ uses $\gamma_n$, between points at $x_c \pm x_m$ looks very small near the zero crossing and larger moving away. The question is, how large are those differences and will they matter for dressing field modulations?

What I first compare is

$$\frac{\omega_{z1} + \omega_{z2}}{\omega_0} \quad (5.11)$$

In Matlab, I take the function

$$f(x) = \text{abs}[J_0(x) - \alpha J_0(\alpha x)] \quad (5.12)$$

and plot it between $x_c - 1$ and $x_c + 1$ with 2000 points on each side of $x_c$ and 1000 points for $x_m$. The difference in their y values are shown in Figure 5.3. Clearly this shows that Equation 5.11 not only increases but increases non-linearly as $x_m$ gets larger. The nEDM experiment will use modulation parameters that can sufficiently offset the pseudomagnetic field, give a large enough scintillation signal and are not too large they give an $\omega_z$ comparable to $\omega_0$.  

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I can expand \( f(x) \) about the point \( x = x_c \) to show the terms that lead to deviations between \( \omega \zeta_1 \) and \( \omega \zeta_2 \) when modulation is symmetric. The derivative of a Bessel function of the first kind can be written as

\[
\frac{\partial J_\nu(z)}{\partial z} = \frac{1}{2} [J_{\nu-1}(x) - J_{\nu+1}(x)]
\]

so that

\[
\begin{align*}
J'_0(x) &= -J_1(x) \\
J''_0(x) &= \frac{1}{2} [J_0(x) - J_2(x)] \\
J'''_0(x) &= -J_1(x) + \frac{1}{2} J_3(x).
\end{align*}
\]

Then I can write \( f(x) \) in Equation 5.12 up to order \( O(x^3) \) as
\[ f(x) \approx \sum_{n=0}^{3} \frac{f^{(n)}(x_c)}{n!}(x - x_c)^n \]

\[
\text{abs}\left[ J_0(x_c) - J_1(x_c)(x - x_c) + \frac{1}{2}[J_0(x_c) - J_2(x_c)] \frac{(x - x_c)^2}{2} + [-J_1(x_c) + \frac{1}{2}J_3(x_c)] \frac{(x - x_c)^3}{6} - aJ_0(ax_c) + aJ_1(ax_c)(x - x_c) - \frac{a}{2}[J_0(ax_c) - J_2(ax_c)] \frac{(x - x_c)^2}{2} - a[-J_1(ax_c) + \frac{1}{2}J_3(ax_c)] \frac{(x - x_c)^3}{6} \right] \\
= \text{abs}\left[ -J_1(x_c)(x - x_c) + \frac{1}{2}[J_0(x_c) - J_2(x_c)] \frac{(x - x_c)^2}{2} + [-J_1(x_c) + \frac{1}{2}J_3(x_c)] \frac{(x - x_c)^3}{6} + aJ_1(ax_c)(x - x_c) - \frac{a}{2}[J_0(ax_c) - J_2(ax_c)] \frac{(x - x_c)^2}{2} - a[-J_1(ax_c) + \frac{1}{2}J_3(ax_c)] \frac{(x - x_c)^3}{6} \right]
\]

(5.15)

Here, \( x = x_c + x_m \). So then looking at \((\omega z_1 - \omega z_2)/\omega_0\) from Equation 5.11 and the results of Equation 5.15 on the following plot
Figure 5.4 Modulating the dimensionless critical dressing condition \( f(x) \) with \( \pm x_m \) and its expansion around the point \( x_c \).

The expansion has simply demonstrated that the first derivative and part of the terms for the second derivative are mostly responsible for the deviations between \( \omega_{z1} \) and \( \omega_{z2} \) around \( x_c \). Furthermore, the same is true if instead \( x_{m1} \neq x_{m2} \) such that \( \omega_{z1} = -\omega_{z2} \).

### 5.2.1.1 The Spin Interaction

The plot of \( \vec{\sigma}_3 \cdot \vec{\sigma}_n \) on critical dressing with no modulations is shown in Figure 5.5. This plot has many frequencies which can be calculated using \( \vec{\sigma}_3(t) \cdot \vec{\sigma}_n(t) \) and the expressions in the previous chapter. However, what is important is the measure of critical dressing, the effect of modulation and the UCN-\(^3\text{He} \) capture rate. Thus, \( \omega_n - \omega_3 \) and \( \omega_n + \omega_3 \) (but more so the former) is desired and averaging out or filtering of larger frequencies could be needed.
Figure 5.5 $\vec{\sigma}_3 \cdot \vec{\sigma}_n$ for critically dressed simulation on the top and a zoomed-in view around 1.0 s on the bottom.

Figure 5.6 shows the fast Fourier transform of $\vec{\sigma}_3 \cdot \vec{\sigma}_n$ shown in Figure 5.5. A few things to note here. First, I’m mostly showing and annotating the greater than 0 frequencies since there’s an equal and opposite frequency of every peak. Second, the total intensity is normalized to 1 and as annotated, the $\omega_3 - \omega_n$ peak has an intensity close to 1. Lastly, the five frequencies larger than $\omega_3 + \omega_n$ come from either the calculation of $\sigma_{x3}\sigma_{xn} + \sigma_{y3}\sigma_{yn} + \sigma_{z3}\sigma_{zn}$ or from anomalous frequencies unaccounted for.
that I discussed in Chapter 4. For instance, the $2\omega$ peak comes from anomalous frequencies. If $\vec{\sigma}_3 \cdot \vec{\sigma}_n$ were to be used for measuring critical dressing, I would want to filter out all the frequencies except $(\omega_3 - \omega_n)$ and maybe $(\omega_3 + \omega_n)$ if I wanted extra accuracy for the fitting. However, fitting $\sigma_x$ for the UCN and $^3$He has proven to be accurate and reliable for finding the critical dressing parameter. Additionally, when it comes to the capture rate that I will see in the $\vec{\sigma}_3 \cdot \vec{\sigma}_n$ plot, the modulations dominate and the large frequencies have no affect.

![Figure 5.6 FFT of $\vec{\sigma}_3 \cdot \vec{\sigma}_n$ showing the many frequencies in Figure 5.5.](image)

For the application of modulations and even though $x_{m1}$ and $x_{m2}$ are the independent variables, in my simulations I start with the basis that

$$< \cos \theta_{n3} > = \frac{\sin \omega_z \tau}{\omega_z \tau},$$

(5.16)

where $\theta_{n3}$ is the angle between the UCN and $^3$He. So I start with setting $\sin \omega_z \tau / \omega_z \tau$ equal to something between 0 and 1 and solving for $\omega_z$ for a given $\tau$. The reason I want to solve for $\omega_z$ first is because my first test is whether the affect of modulation is appropriately labeled as a relative frequency difference about the $z$-axis. For instance, if I start with the following parameters
Figure 5.7 Three dimensional plot of $\sigma_x$, $\sigma_y$ and time with modulation. The separation between the $^3He$ in red and UCN in blue shows poor modulation created a relative phase.

$$< \cos \theta_{n3} > = \frac{\sin \omega_z \tau}{\omega_z \tau} = 0.50$$

$$\tau = 0.40 \text{ s}$$

$$\rightarrow \omega_z = 4.7387 \text{ rad/s}$$

$$B_0 = 3 \cdot 10^{-6} T, \quad y = 1/10 \quad x_c = 1.1824619208064,$$

$x_{m1,2}$ can be solved for

$$0 = J_0(x_c + x_{m1}) - \alpha J_0(\alpha(x_c + x_{m1})) - \frac{\omega_z}{\gamma_n B_0}$$

$$0 = J_0(x_c - x_{m2}) - \alpha J_0(\alpha(x_c - x_{m2})) + \frac{\omega_z}{\gamma_n B_0}$$

$$\rightarrow x_{m1} = 0.061554, \quad x_{m2} = 0.049009.$$  

These values lead to $\vec{\sigma}_3 \cdot \vec{\sigma}_n$ being quite asymmetric. Figure 5.7 shows the last 1.0% of the simulation and is a three dimensional plot of $< \sigma_x, \sigma_y, t >$ for Helium in red and UCN in blue. The separation between the red and blue demonstrates a phase shift has been created. The modulation is doing a poor job.
Figure 5.8 $\vec{\sigma}_3 \cdot \vec{\sigma}_n$ vs time with same parameters as Figure 5.7.

Additionally, Figure 5.8 shows the same parameters used in Figure 5.7 but for $\vec{\sigma}_3 \cdot \vec{\sigma}_n$ vs time. The large asymmetry in $x_{m1,2}$ is leading to a quick and large phase shift. The next section will investigate why symmetric $\omega_z$ is leading to asymmetry in $\vec{\sigma}_3 \cdot \vec{\sigma}_n$. For reference, Figure 5.9 shows $<\sigma_x, \sigma_y, t>$ for the last 1.0% of the simulation for critical dressing without modulation.
Figure 5.9 Three dimensional plot of $\sigma_x$, $\sigma_y$ and time with no modulation and critical dressing. The blue and red curves stay on top of each other. It's hard to see without projecting into the $\sigma_x$-t or $\sigma_y$-t plane but there is essentially no separation between the spin directions of UCN and Helium.

5.2.2 Third Order Corrections to the Eigenvalues

There is a choice of either symmetric $x_m$, symmetric $\omega_z$ or neither. Through experimenting using my RK4, a symmetric $x_m$ was leading to a smaller phase difference between the $^3$He and UCN. This can be seen in Figure 5.10 where I start the two species perpendicular to each other. In blue is when there is symmetric $\omega_z$ but asymmetric $x_m$. Orange, yellow and purple are symmetric $x_m$ and asymmetric $\omega_z$. There's a phase shift building on the blue curve. Whereas the other curves are close to symmetric about 0, the starting point.
So is the definition of $\omega_z$ not a precession solely about the z-axis? Instead, it’s possible that the effect of modulation also causes a change to $\omega_x$ and therefore $\omega_z$ is instead a vector $\vec{w}_{x,z}$ (there’s no field along the y-axis so there’s no outright $\omega_y$).

For testing if $\omega_z$ isn’t a frequency solely around the z-axis, I performed some simple simulations. For instance, if $x_c$ is simply shifted to $x_c + x_m$ for an entire simulation, does the $\omega_{n3} = \omega_z$? When I did this for my usual parameters, the answer was no. But if I changed y from 0.10 to 0.005, the answer was yes indicating there may be a dependence on y. In one simulation with $B_0 = 3 \cdot 10^{-7}$T, $x = x_c + x_m = 1.189018 + 0.004$ and $y = 0.005$, fitting each $\sigma_x(t)$ I had

$$\omega_n - \omega_3 = 0.0344146$$
$$\omega_z = -B_0 \gamma_n [ J_0(x) - \alpha J_0(\alpha x)] = 0.0343269.$$

Given this and the fact that for any $y$, symmetric $x_m$ modulation led to near symmetry for $\vec{\sigma}_3 \cdot \vec{\sigma}_n$, I turned to the fact that my simulations with $y = 0.10$, as well as in the nEDM experiments, are not sufficiently in the $J_0$ approximation. Hence, the first issue is that Equation 5.4 is only valid for $y << 1$ and more terms are needed to test if $\vec{\sigma}_3 \cdot \vec{\sigma}_n$ is symmetric for modulations of symmetric $\omega_z$ and $y = 0.10$. Then I can appropriately test for whether symmetric $\omega_z$ means symmetry about the x-y plane.

As previously shown, the $J_0$ approximation is actually just using the first order correction to the eigenvalues that lifted the degeneracy. When it comes to the second order correction, not only did I not see a contribution in the Fourier transforms of the individual spins but in my search for the anomalies, I
calculated that it summed to 0. The general expression for the second order correction to the eigenvalues is

$$E^{(2)}(\lambda) = \lambda^2 \sum_{k \neq n} \frac{|\langle k^{(0)} | V | n^{(0)} \rangle|^2}{E_n^{(0)} - E_k^{(0)}},$$

(5.20)

and using the bar eigenstates of $m_z$ where $m_z = \pm \frac{1}{2} = \pm \frac{m}{2}$

$$E^{(2)} = \frac{\omega_0^2}{4} \sum_{n' m'} \frac{|\langle n', m' | \sigma_z | n, m \rangle|^2}{(n - n')\omega} = y \frac{\omega_0}{16} \sum_{n', q \neq 0} \frac{[m J_q(x)(-1)^q + m' J_q(x)]^2}{q} = 0.$$

(5.21)

Next are the third order corrections to the eigenvalues which I suspected to be the source. Based off the Swank [CS18] paper, the deviation of $x_c$ away from the limit depends on $y^2$ and the third order corrections will be proportional to $y^2$. This can be seen in Figure 5.11.

![Figure 5.11 Difference between effective $x_c$ and limit $x_c$](image)

**Figure 5.11** Difference between $x_c$ found using simulations and $x_c$ found in the $J_0$ approximation from the Swank, Webb, Liu, Filippone paper [CS18]

The third order corrections to the eigenvalues have two summation terms and one is easier to calculate than the other. The general expression is

$$E_n^{(3)} = \sum_{k \neq n} \sum_{m \neq n} \frac{\langle n^{(0)} | V | m^{(0)} \rangle \langle m^{(0)} | V | k^{(0)} \rangle \langle k^{(0)} | V | n^{(0)} \rangle}{(E_n^{(0)} - E_m^{(0)})(E_n^{(0)} - E_k^{(0)})} - \langle n^{(0)} | V | n^{(0)} \rangle \sum_{m \neq n} \frac{|\langle n^{(0)} | V | m^{(0)} \rangle|^2}{(E_n^{(0)} - E_m^{(0)})^2}. $$

(5.22)
so that I can write the third order correction in this context as

\[
P_n^{(3)} = \sum_{n',m' \neq n,m} \sum_{n''} \frac{\langle n,m | \frac{1}{2} \omega_0 \sigma_z | n'',m'' \rangle \langle n'',m'' | \frac{1}{2} \omega_0 \sigma_z | n',m' \rangle \langle n',m' | \frac{1}{2} \omega_0 \sigma_z | n,m \rangle}{(n\omega - n''\omega)(n\omega - n'\omega)}
\]

\[
= \frac{1}{2} \omega_0 |J_0(x) + mJ_0(x)| \sum_{n',m'} \left\lfloor \frac{|\langle n',m' | \frac{1}{2} \omega_0 \sigma_z | n,m \rangle|^2}{(n\omega - n'\omega)^2} \right\rfloor
\]

\[
= -\frac{\omega_0}{4} [mJ_0(x) + mJ_0(x)] \sum_{q,m'} \left\lfloor \frac{|mJ_q(x)(-1)^q + m'J_q(x)|^2}{(q\omega)^2} \right\rfloor
\]

\[
= -\frac{1}{32} m\omega_0 J_0(x) y^2 \sum_{q,m'} \left\lfloor \frac{|mJ_q(x)(-1)^q + m'J_q(x)|^2}{q^2} \right\rfloor
\]

\[
\sum_{m'=\pm m} \left[ \frac{[-mJ_1(x) + m'J_1(x)]^2}{(1)^2} + \frac{[mJ_1(x) - m'J_1(x)]^2}{(1)^2} + \frac{[mJ_2(x) + m'J_2(x)]^2}{(2)^2} + \frac{[mJ_2(x) + m'J_2(x)]^2}{(2)^2} + \frac{[mJ_3(x) + m'J_3(x)]^2}{(3)^2} + \frac{[mJ_3(x) - m'J_3(x)]^2}{(3)^2} + \ldots \right],
\]

so that the result is

\[
= -\frac{1}{4} m\omega_0 J_0(x) y^2 \left[ J_1^2(x) + \frac{J_2^2(x)}{4} + \frac{J_3^2(x)}{9} + \ldots \right]
\]

\[
= -\frac{1}{2} m z \omega_0 J_0(x) y^2 \left[ J_1^2(x) + \frac{J_2^2(x)}{4} + \frac{J_3^2(x)}{9} + \ldots \right].
\]

The Physics Reports [Gol94] made the approximation that the first term, which is more complicated than the second, is equal in magnitude as the second term and therefore did not calculate it. What I found is that the first term is actually larger than the second term and when included in the critical dressing condition, produces much better convergence with simulation values. The calculation for the second term is

\[
= -\frac{1}{32} m\omega_0 J_0(x) y^2 \sum_{q,m'} \left\lfloor \frac{|mJ_q(x)(-1)^q + m'J_q(x)|^2}{q^2} \right\rfloor
\]

such that for different \( q \)'s, \( m' = m \) or \( m' \neq m \). The terms up to \( J_3(x) \) are

\[
\sum_{m'=\pm m} \left[ \frac{[-mJ_1(x) + m'J_1(x)]^2}{(1)^2} + \frac{[mJ_1(x) - m'J_1(x)]^2}{(1)^2} + \frac{[mJ_2(x) + m'J_2(x)]^2}{(2)^2} + \frac{[mJ_2(x) + m'J_2(x)]^2}{(2)^2} + \frac{[mJ_3(x) + m'J_3(x)]^2}{(3)^2} + \frac{[mJ_3(x) - m'J_3(x)]^2}{(3)^2} + \ldots \right],
\]

so that the result is

\[
= -\frac{1}{4} m\omega_0 J_0(x) y^2 \left[ J_1^2(x) + \frac{J_2^2(x)}{4} + \frac{J_3^2(x)}{9} + \ldots \right]
\]

\[
= -\frac{1}{2} m z \omega_0 J_0(x) y^2 \left[ J_1^2(x) + \frac{J_2^2(x)}{4} + \frac{J_3^2(x)}{9} + \ldots \right].
\]

For the calculation of the first term in Equation 5.23, first I would like to consider the terms that contain \( J_0(x) \) since they will be similar in magnitude to the result in Equation 5.26. The only way to get a \( J_0(x) \) in the first term is for \( m = k \) which means \( n' = n'' \) (but with \( m' = \pm m'' \)) giving
The summation over $m'$ made $m'' = m'$ or else the whole term vanishes. Continuing the calculation of just the sum

$$\sum_{m',q \neq 0} \frac{m'[mJ_q(x)(-1)^q + m'J_q(x)]^2}{q^2}$$

$$= \sum_{m'} \left[ m'[-mJ_1(x) + m'J_1(x)]^2 + \frac{m'[mJ_1(x) - m'J_1(x)]^2}{2} + \frac{m'[mJ_2(x) + m'J_2(x)]^2}{(-2)^2} + \frac{m'[mJ_3(x) + m'J_3(x)]^2}{3^2} + \frac{m'[mJ_4(x) - m'J_4(x)]^2}{(-3)^2} + \ldots \right]$$

$$= \left[ \frac{-16m^3J_1^2(x)}{1} + \frac{16m^3J_2^2(x)}{4} + \frac{-16m^3J_3^2(x)}{9} + \ldots \right].$$

(5.28)

The summation over $m'$ is simply a summation of $m' = m$ and $m' = -m$. Then substituting $m = 2m_z$ as before, the final result for the first term in Equation 5.23 is

$$\frac{1}{32} \omega_0 I_0(x) y^2 \sum_{m',m'' \neq 0} \frac{[mJ_q(x)(-1)^q + m'J_q(x)]^2 [m' + m'']}{q^2}$$

$$= m_z \omega_0 I_0(x) y^2 \left[ -J_1^2(x) + \frac{J_2^2(x)}{4} - \frac{J_3^2(x)}{9} + \ldots \right].$$

(5.29)

The new critical dressing condition is
\[(\omega_0 - \omega_3) = 0 = (-\gamma B_0) \left[ J_0(x_c) - a J_0(a x_c) \right] \]
\[-J_0(x_c) \frac{y^2}{2} \left[ J_1^2(x_c) + \frac{J_2^2(x_c)}{4} + \frac{J_3^2(x_c)}{9} + \ldots \right] + a^3 J_0(a x_c) \frac{y^2}{2} \left[ J_1^2(a x_c) + \frac{J_2^2(a x_c)}{4} + \frac{J_3^2(a x_c)}{9} + \ldots \right] + J_0(x) y^2 \left[ -J_1^2(x_c) + \frac{J_2^2(x_c)}{4} - \frac{J_3^2(x_c)}{9} + \ldots \right] + a^3 J_0(x_c) y^2 \left[ -J_1^2(a x_c) + \frac{J_2^2(a x_c)}{4} - \frac{J_3^2(a x_c)}{9} + \ldots \right] \]

\[
= (-\gamma B_0) \left[ J_0(x_c) - a J_0(a x_c) \right] - J_0(x_c) \frac{y^2}{2} \left[ 3J_1^2(x_c) - \frac{3J_2^2(x_c)}{4} + \frac{3J_3^2(x_c)}{9} + \ldots \right] + a^3 J_0(a x_c) \frac{y^2}{2} \left[ 3J_1^2(a x_c) - \frac{3J_2^2(a x_c)}{4} + \frac{3J_3^2(a x_c)}{9} + \ldots \right].
\]

(5.30)

Now, going back to the other terms that do not include \(J_0(x)\), they will either vanish when summed over or be quite small. For example, the next terms would have \(n' - n'' = \pm 1\) and some example values could be \(n' = 2\) and \(n'' = 1\). This means \(n \neq 1, 2\) so that the smallest \(q\) and \(q'\) available is for \(n = 0\) or \(n = 3\). Generally

\[
\frac{(n, m|\sigma_z|n'', m'')(n'', m'')|\sigma_z|n', m')\langle n', m'|n, m \rangle}{(n - n')\omega(n - n'')\omega} = \frac{1}{8} \left[ m'' J_{-q'}(x)(-1)^{-q'} + m J_{-q'}(x) \right] \left[ m' J_{q''}(x)(-1)^q + m'' J_{q''}(x) \right] \frac{m J_q(x)(-1)^q + m' J_q(x)}{(q\omega)(q'\omega)}.
\]  

(5.31)

The two cases above will yield the following terms

\[
n' = 2, n'' = 1, n = 0
q = 2, q' = 1, q'' = 1
\]

\[
\frac{1}{8} \left[ m'' J_1(x) - m J_1(x) \right] \left[ -m' J_1(x) + m'' J_1(x) \right] \frac{m J_2(x) + m' J_2(x)}{(2\omega)(1\omega)} = \frac{m J_1^2(x) J_2(x)}{2\omega^2}
\]  

(5.32)

\[
n' = 2, n'' = 1, n = 3
q = -1, q' = 2, q'' = 1
\]

\[
\frac{1}{8} \left[ m'' J_2(x) + m J_2(x) \right] \left[ -m' J_1(x) + m'' J_1(x) \right] \frac{m J_1(x) - m' J_1(x)}{(-1\omega)(2\omega)} = \frac{-m J_1^2(x) J_2(x)}{2\omega^2},
\]

where certain conditions had to be chosen to avoid 0. In the first case: \(m'' = -m', m'' = m \rightarrow m'' = -m\).
Figure 5.12 Solutions for critical dressing parameters for different $Y = 1/y$ with the third order corrections as part of the condition. The first line in the legend is just a vertical line for $x = 1.189018$, the solution for critical dressing in the $J_0$ approximation.

And for the second case: $m'' = -m', m' = -m \rightarrow m'' = m$. The two results in Equation 5.30 sum to 0. Many terms throughout this sum will cancel each other out. The ones that do not will be small enough relative to the $J_0(x)$ terms to only cause small errors as can be seen in plots below.

Figure 5.12 shows the zoomed-in view of the new critical dressing condition and how $x_c$ varies for different values of $y$. This demonstrates how the nEDM experiments needs to account for this shift in $x_c$ not only for the sake of critical dressing and modulating the dressing field but for an accurate expression for the scintillation rate. This third order correction also dilutes the nEDM signal.
What I now see from my simulations is much better agreement between my simulation $x_c$ and the analytical expression for $x_c$ that includes the third order corrections. Figure 5.13 shows the analytical and simulation $x_c$’s for different values of $y$. And Figure 5.14 shows the percentage difference of these values at each given value of $y$. For $y = 0.10$, my percent difference went from $\approx -1.5\%$ to $\approx -0.02\%$ after I included the first term in Equation 5.21. There is still a $y^2$ dependence in Figure 5.14 because the third order correction terms I’ve ignored are of course still proportional to $y^2$. Given I now have an accurate expression for the critical dressing condition, I can more accurately modulate around it.
5.3 RK4 Results

5.3.1 Modulations and Symmetric Spin Interaction

What the last subsection taught me was that $\vec{\sigma}_3 \cdot \vec{\sigma}_n$ showed good symmetry for $x_{m1} = x_{m2}$ and $\omega_z1 \neq -\omega_z2$ not necessarily because the modulation's affect is outside the x-y plane but because the $\omega_z$ expression I was using was incorrect. Now with the third order corrections, I will go back to each case and see how it effects $\vec{\sigma}_3 \cdot \vec{\sigma}_n$. I will also do it for the initial condition that the spins are parallel because this will be how the experiment starts and it also will show the scintillation signal more clearly.

To start, I will note that there is still an inconsistency that will only be resolved with more terms for the third order corrections and possibly higher order corrections. It comes from the fact that in solving for $x_{m1,2}$, an $x_c$ is required. I can either use the analytical value or the simulation value (for a given $B_0$ and $y$). If I choose $\omega_{z1} = -\omega_{z2}$ and use the analytical $x_c$, inputting the $x_m$'s into the simulation will yield unequal $\omega_z$'s because the simulation uses a different $x_c$. Whereas, if I used the simulation $x_c$ to solve for the $x_m$'s, there's still a small error given $y = 0.10$ does not pair with the simulation $x_c$. This can be seen in Figure 5.15 where there's no symmetry for $x_m$ and $\omega_z$ and the $\vec{\sigma}_3 \cdot \vec{\sigma}_n$ signals look somewhat symmetric. This was because $x_{m1}$ and $x_{m2}$ were solved for using the analytical $x_c$. There is not good symmetry for $\vec{\sigma}_3 \cdot \vec{\sigma}_n$. 

![Figure 5.14](image-url) The percentage difference between points in Figure 5.13 for a given $Y$. 

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The next case is for $x_{m1} = x_{m2}$. This can be seen in Figure 5.16 and clearly there's a phase shift building for $\omega_{z1}$ modulations vs. $\omega_{z2}$ modulations. Hence, this modulation would do a poor job canceling out the pseudomagnetic field.
Finally, for the case where \( \omega_{z1} = -\omega_{z2} \), the symmetry for the scintillation signal in \( \sigma_3 \cdot \sigma_n \) was possibly the best for the three cases. It’s shown in Figure 5.17. One thing is clear: \( \omega_{z1} \) nearly equal to |\( \omega_{z2} \)| gave better results. This can be indicative that \( \omega_{z1} = -\omega_{z2} \) is the solution we want for a symmetric scintillation signal.
Of the three cases I showed, \( x_{m1} \neq x_{m2} \) and \( \omega_{z2} \neq -\omega_{z1} \) had the best symmetry. But improvement is still needed before incorporating a pseudomagnetic field. There were a few things I tried to help bring more symmetry to the scintillation signal. First, I can be asymmetric in \( \tau \): use a \( \tau_1 \) and \( \tau_2 \). So I can take a curve like in Figure 5.16, and try to compensate for the difference between \( \omega_{z1,2} \) using \( \tau_1 = 0.19 \) s and \( \tau_2 = 0.20 \) s instead of \( \tau = 0.20 \) s for both modulations. This had an odd affect and did not bring more symmetry in the slightest. Second, I can still use \( \tau_1 = \tau_2 \) but have the first modulation be shorter: \( \tau'/2 \). For instance, instead of a \( \tau/2 \) lasting for 0.10 s, modulation for \( \tau'/2 = 0.075 \) s. However, this essentially flipped the asymmetry around and can be seen in Figure 5.18.

**Figure 5.17** \( \sigma_3 \cdot \sigma_n' \) vs time for the last case, symmetric \( \omega_z \).
Figure 5.18 $\sigma_3 \cdot \sigma_n$ vs time with symmetric $x_m$ modulation but the first $x_{m1}$ modulation lasting for 0.075 s instead of 0.10 s.

Lastly, I can increase or decrease $\tau$ for the sake of decreasing whatever asymmetry exists in the phase shifts and then experiment via trial and error with $x_{m1,2}$. I then start with the script that takes an $x_c = 1.182461920806400$, $\tau = 0.40 s$ and $B_0 = 30 mG$ as inputs and I set $\sin \omega_z \tau / \omega_z \tau = 0.50$ then solve for $x_{m1,2}$. I can loop through different values of $x_{m1}$ to see which gives the best symmetry for $\sigma_3 \cdot \sigma_n$. I test for this symmetry by finding the minimums of $\sigma_3 \cdot \sigma_n$ (scintillation signals) near $\tau / 2$ points and then calculate the standard deviation. Where I started looping through $x_{m1}$ and what the constant $x_{m2}$'s were, was based off what my script first solved for given the mentioned inputs. The table summarizing these results is shown in Table 5.1. Then for the lowest standard deviation, the plot of $\sigma_3 \cdot \sigma_n$ using these parameters is shown in Figure 5.19.
Table 5.1 Starting from an $x_m$ pair that gave decent $\vec{\sigma}_3 \cdot \vec{\sigma}_n$ symmetry, I looped through 10 values of $x_{m1}$ around the original and kept $x_{m2}$ constant. I then recorded the standard deviation of the minimum $\vec{\sigma}_3 \cdot \vec{\sigma}_n$ at each scintillation signal (trough). $x_{m1} = 0.0555$ and $x_{m2} = 0.056107$ had the lowest standard deviation.

<table>
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<tr>
<th>$x_{m1}$</th>
<th>$x_{m2}$</th>
<th>$\vec{\sigma}_3 \cdot \vec{\sigma}_n$ signal standard deviation</th>
</tr>
</thead>
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<tr>
<td>0.0550</td>
<td>0.056107</td>
<td>0.0222</td>
</tr>
<tr>
<td>0.0551</td>
<td>0.056107</td>
<td>0.0181</td>
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<td>0.056107</td>
<td>0.0139</td>
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</tr>
<tr>
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<td>0.056107</td>
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<td>0.056107</td>
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<tr>
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</tr>
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</tr>
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</tr>
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</tr>
<tr>
<td>0.0560</td>
<td>0.056107</td>
<td>0.0205</td>
</tr>
</tbody>
</table>

Figure 5.19 $\vec{\sigma}_3 \cdot \vec{\sigma}_n$ vs time for modulation parameters $x_{m1} = 0.0555$ and $x_{m2} = 0.056107$. The scintillation signals are more symmetric than any other modulated $\vec{\sigma}_3 \cdot \vec{\sigma}_n$ plot I have shown.

This $\vec{\sigma}_3 \cdot \vec{\sigma}_n$ is close to symmetric and what I will use when incorporating a pseudomagnetic field. Note
that \( \omega_{z1} \) is close to \(-\omega_{z2} \) but they do differ by a non-negligible amount. I think what I’m seeing is that \( \omega_{z1} = -\omega_{z2} \) does bring symmetry to \( \vec{\sigma}_3 \cdot \vec{\sigma}_n \) but the values I calculate are still missing enough corrections to the eigenvalues to produce a 1% difference.

### 5.3.2 Applying a Pseudo Magnetic Field

Given I have a reasonably modulated time series for \( \vec{\sigma}_3 \cdot \vec{\sigma}_n \), I can apply a pseudomagnetic field, \( \vec{P} \). First, I’ll look at how \( \vec{P} \) affects \( \vec{\sigma}_3 \cdot \vec{\sigma}_n \) without any modulations. And then whether the modulations can sufficiently offset \( \vec{P} \)’s effects.

For the implementation of \( \vec{P} \), ordinarily there would need to be an ensemble and spatial average over \(^3\)He particles for a proper representation. However, given my simulations use one particle since the fields are independent of position and velocity, I can simply align \( \vec{P} \) along the \(^3\)He spin angles. Furthermore, since \( S^2 \) is normalized to 1 on the Bloch sphere, I can literally use the \(^3\)He spin components for the pseudomagnetic field then multiply by the fields magnitude. This can be written as

\[
P_x = |\vec{P}|\sigma_{3x}, \quad P_y = |\vec{P}|\sigma_{3y}, \quad P_z = |\vec{P}|\sigma_{3z}.
\]  

(5.33)

One issue is an averaging procedure is required to give the pseudomagnetic field twice the elements as the spins so that it can be used in the RK4. So I took each pair of elements created in Equation 5.33 and inserted the average of the pair between them. Once \( \vec{P} \) is constructed after the first half of the simulation that dealt with the \(^3\)He, I add \( P_i \) to each total magnetic field component for the UCN half.

For the magnitude of \( \vec{P} \), I’ll use the value from the paper by Leung et al.[Leu19] where for \( x_3 = 10^{-10} \) and \( P_3 = 1: |\vec{P}| \approx 0.10 \mu G \). However, this magnitude is very small compared to the fields already present so instead I looked at \( |\vec{P}| \approx 10 \mu G \) and \( 50 \mu G \). The plots of each field in different scenarios is shown in Figures 5.20 to 5.25. For each pseudomagnetic field, I first show the difference in \( \vec{\sigma}_3 \cdot \vec{\sigma}_n \) for the field off and on without modulation. Followed by plots where modulation will cancel out the effects from \( \vec{P} \). Note that in Figures 5.20 and 5.23, I chose to use the color blue for the pseudomagnetic field on and orange for it off which differs from other plots. This was solely to give a better contrast to the naked eye.
Figure 5.21 $\sigma_3 \cdot \sigma_n$ vs time with modulation and the pseudomagnetic field off (blue) and on (orange). The magnitude of $\vec{P}$ is about 100 times larger than in the experiment.

Figure 5.20 $\sigma_3 \cdot \sigma_n$ vs time for no modulation and the pseudomagnetic field off (orange) and on (blue). The magnitude of $\vec{P}$ is about 100 times larger than in the experiment.
Figure 5.20 showed that $\vec{P}$ was inducing a non-negligible phase shift between the $^3$He and UCN that grows linear in time (with no modulation). Then Figures 5.21 and 5.22 show the modulation doing a good job at canceling the phase difference that was built in the plots without modulation. The mean of the difference between the pseudomagnetic field on and off in Figure 5.21 is 0.000317 with a standard deviation 0.00237. Table 5.2 shows the mean and standard deviation between curves with $\vec{P}$ on and off for six pseudomagnetic field strengths with modulation on. Their respective plots are shown in Figures 5.27 and 5.28.

Figure 5.22 A zoomed-in view of Figure 5.21 near 1.0 s.
Figure 5.24 $\vec{\sigma}_3 \cdot \vec{\sigma}_n$ vs time with modulation and the pseudomagnetic field off (blue) and on (orange). The magnitude of $\vec{P}$ is about 500 times larger than in the experiment.

Figure 5.23 $\vec{\sigma}_3 \cdot \vec{\sigma}_n$ vs time for no modulation and the pseudomagnetic field off (orange) and on (blue). The magnitude of $\vec{P}$ is about 500 times larger than in the experiment.
Figure 5.25 A zoomed-in view of Figure 5.24.

Table 5.2 For the pseudomagnetic field off and on curves in Figure 5.21, I calculated the mean distance between each curve at a given time point and the standard deviation of that data. Then did it for six pseudomagnetic field magnitudes.

| \(|\vec{B}| (\mu \text{G})\) | Mean Distance Between Curves | Standard Deviation of Distances |
|-----------------------------|-----------------------------|-------------------------------|
| 0.10                        | 0.000000844                 | 0.0000238                     |
| 0.50                        | 0.00000468                  | 0.000119                      |
| 1.00                        | 0.0000105                   | 0.000238                      |
| 5.00                        | 0.0000981                   | 0.00119                       |
| 10.00                       | 0.000317                    | 0.00237                       |
| 50.00                       | 0.00702                     | 0.0136                        |
Figure 5.26 The mean data from Table 5.2 plotted with log axes.

Figure 5.27 The standard deviation data from Table 5.2 plotted with log axes.
The relationship between mean distance and pseudomagnetic field strength in Figure 5.26 is higher order than linear but not quite quadratic. Whereas the relationship in Figure 5.27 is linear. Given the very small value of mean distance between curves for $|\vec{P}| = 0.10 \mu G$, modulation in the nEDM experiment should sufficiently offset the effects of $\vec{P}$.

After discussing the significance of these plots with Bob, he had the idea to check the relationship between the first and second harmonic signals in Fourier space. The idea is that the first harmonic at 1.25 Hz should be near zero if the modulations are symmetric about $x_c$. Whereas the second harmonic will have a much larger height and increase in height as the first harmonic signal decreases. So checking the ratio of the second to the first harmonic with modulation on pseudomagnetic field off and modulation on pseudomagnetic field on, will be a better test of whether the modulations are doing their job. My results from Table 5.1 where I chose the $x_{m1}$ and $x_{m2}$ that give the lowest standard deviation between scintillation signals actually were close to what this new method gave. I optimized symmetry by looping through $x_{m1}$ values that produced the lowest first harmonic signal. The results were $x_{m1} = 0.05546$ and $x_{m2} = 0.056107$ and I used a simulation time of 8 seconds. Figure 5.28 shows $\sigma_3 \cdot \sigma_n$ with modulations on, pseudomagnetic field off using these new parameters and Figure 5.29 shows the FFT of Figure 5.28 but zoomed on the modulation harmonics.

With the first harmonic very small, I ran simulations with the pseudomagnetic field on with a strength of 10 $\mu G$ and compared the ratios of heights between the second and first harmonics. First shown in Figure 5.30 is $\sigma_3 \cdot \sigma_n$ with the pseudomagnetic field off (blue) and on (orange) and a zoomed-in view of a maximum scintillation signal at 5.40 s.
The FFT of Figure 5.28 zoomed-in on the harmonics.

The FFTs are shown in Figure 5.31 where I zoomed-in on the first harmonics but further zoomed-in on the first (1.25 Hz) and second (2.5 Hz) harmonics. The colors have been changed to better see where the curves differ and overlap.
The black curve for when the pseudomagnetic field is on has a larger value at the first harmonic which is expected. Due to the binning of the frequency axis which comes from the time steps and length of the simulation, there was no value exactly on 1.25 Hz or 2.5 Hz. For the 1.25 Hz, I took the average of the values at 1.1875 Hz and 1.3125 Hz. For the 2.5 Hz, I used the value at 2.4375 Hz. The results were that the ratio of the second harmonic signal to the first with the pseudomagnetic field off was 30.055. The ratio with the pseudomagnetic field on was 13.346. Thus, the pseudomagnetic field being flipped to on changed the relative ratios by about a factor of 2.25. This change is a good benchmark as to how well the modulations do going forward and with a field that is not 100x the experiment’s strength. Additionally, Figure 5.32 shows the same FFT as Figure 5.31 but just the curve with the pseudomagnetic field off and an averaging procedure done. I took every 1000 points and found the average which created a new point in the new data.

**Figure 5.32** Zoomed-in view of the first harmonic after averaging data into 1000 data point bins.

As seen, the first harmonic has a minimum achieved through proper choosing of the modulation parameters and the ratio of the second to first harmonic is amplified.
Figure 5.30 $\sigma_3 \cdot \sigma_n$ modulated with a 10 $\mu$G pseudomagnetic field shown in the orange curve.
Figure 5.31 The first and second harmonics. Their ratios are an indicator of how well modulation is working.
The conclusions I have drawn from my research are the following:

From Chapter 3, ComSol solved the spin Bloch Equations well enough for its solver to continue being used. The test of whether it was able to match with theory from [ALB06] and [GP15] was successful. For the former, the gas collisions expressions actually matched with ComSol’s no gas collision simulations the best. Albeit with the parameter $r_0$ small, meaning very little gas collisions would take place. It would be interesting to incorporate gas collisions to mimic $^3$He particle dynamics and see how they compare to the Barabanov numerical data for $r_0$ values that are not small. For the comparison to Pignol adiabatic and non-adiabatic expressions, the circle cases were hit or miss whereas the rectangle did quite well. Furthermore, Pignol derived those results for three dimensional geometries and some assumptions so taking ComSol simulations to three dimensions would be a better comparison. Three dimensional simulations can take time for thousands of particles but the results from the rectangle are promising. And even with potentially more accurate solvers, like my RK4 but which takes longer than ComSol to handle thousands of particles, the use of ComSol for ballistic or diffuse scattering gas collision trajectories is very useful.

In Chapter 4 I showed that when I used my RK4 solver to solve the spin Bloch Equations for dressed spins as functions of time and then perform FFTs of these time series, there were anomalous frequencies not accounted for in the theory from [Gol94]. Additionally, I showed that a different method which constructs and diagonalizes the Hamiltonian showed the same anomalies in the spin components. Finally, I used first order perturbation theory to find the first order corrections to the eigenstates that are linear in the perturbation strength $y$. When summing over spins and $q$’s, the non-vanishing terms gave results with frequencies matching the anomalous frequencies. Even though incorporating the
new theoretical terms into the plots with the RK4 results showed a difference in peak heights, those differences can probably be drawn back to missing Bessel function terms or normalization issues. To extract $\omega_3 - \omega_n$ for the scintillation rate, a low-pass filter will be needed for the $^3$He-UCN interaction term such that high frequencies including the anomalies will not contribute. In the future, there are still the second order corrections I can solve for to account for an anomaly like the $\omega$ frequency in $\sigma_x$. Furthermore, it would be interesting to see how the third order corrections to the eigenvalues in Chapter 5 affect the anomaly locations since the corrections would go into the time evolution operator and shift the energies, although by a very small amount. (But this small amount was very important for the sensitive critical dressing condition.)

In Chapter 5, the goal was to create and implement a way to modulate the dressing field such that the pseudomagnetic field’s effect can be averaged out of the simulations and therefore the experiment. But before getting to pseudomagnetic field, I saw that modulating the dressing field and therefore the capture rate seen in $\vec{\sigma}_3 \cdot \vec{\sigma}_n$ was not straightforward. There were large asymmetries for different modulation parameters. Not only this but the critical dressing parameter which the modulation parameter $x_m$ is added or subtracted from has always been different between my simulations and the analytical solution. I found that there should be a difference because $y = 0.10$ is not small enough for the $J_0$ approximation to hold. Given that, I solved for the third order correction to the eigenvalues so that the critical dressing condition was more valid for $y = 0.10$. Then I was able to modulate better and find a modulation that gave good symmetry for the scintillation signals. The nEDM experiment will use $y = 0.10$ so it is very important for the spin dressing measurement mode to use the correct value of the dressing parameter given the third order correction I have detailed. Finally, I showed that the modulations were doing a good job at offsetting the pseudomagnetic field. What can be done in the future is to have an ensemble of $^3$He particles diffusing in a trap, solving for the pseudomagnetic field and performing modulation on it.
BIBLIOGRAPHY


APPENDIX
A.1 A1

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439/216 & -8320/216 & 7296/2197 & 0 & 0 \\
-8/27 & 2 -3544/2565 & 1859/4104 & -11/40 & 0 \\
0 & 3600/513 & -845/4104 & 0 & 0 \\
-355/3744 & 0 & 3600/513 & -845/4104 & 0 \\
901/3600 & -2187/4104 & 355/1296 & 0 & 0 \\
0 & 7296/2197 & 3600/513 & -845/4104 & 0 \\
-4387/216 & 0 & 7296/2197 & -845/4104 & 0 \\
696/35 & -230& 0 & 7296/2197 & 0 \\
9208/2197 & -845/36 & 7296/2197 & -845/4104 & 0 \\
-845/182 & 0 & 7296/2197 & -845/4104 & 0 \\
-845/182 & 0 & 7296/2197 & -845/4104 & 0
\end{bmatrix}
\]

CH = \[
\begin{bmatrix}
16/135; 0; 6656/12825; 28561/56430; -9/50; 2/55
\end{bmatrix}
\]

for M=1:N
for i=1:tn-1

k1x = dSxdt(Sy(M,i),Sz(M,i),ByN(M,i),BzN(M,i));
k1y = dSydt(Sx(M,i),Sz(M,i),BxN(M,i),BzN(M,i));
k1z = dSzdt(Sx(M,i),Sy(M,i),BxN(M,i),ByN(M,i));

k2x = dSxdt(Sy(M,i)+B(2,1)*h*k1y,Sz(M,i)+B(2,1)*h*k1z,ByN(M,i),BzN(M,i));
k2y = dSydt(Sx(M,i)+B(2,1)*h*k1x,Sz(M,i)+B(2,1)*h*k1z,BxN(M,i),BzN(M,i));
k2z = dSzdt(Sx(M,i)+B(2,1)*h*k1x,Sy(M,i)+B(2,1)*h*k1y,BxN(M,i),ByN(M,i));

k3x = dSxdt(Sy(M,i)+B(3,1)*h*k1y+B(3,2)*h*k2y,Sz(M,i)+B(3,1)*h*k1z +B(3,2)*h*k2z,ByN(M,i),BzN(M,i));
k3y = dSydt(Sx(M,i)+B(3,1)*h*k1x+B(3,2)*h*k2x,Sz(M,i)+B(3,1)*h*k1z +B(3,2)*h*k2z,BxN(M,i),BzN(M,i));
k3z = dSzdt(Sx(M,i)+B(3,1)*h*k1x+B(3,2)*h*k2x,Sy(M,i)+B(3,1)*h*k1y +B(3,2)*h*k2y,BxN(M,i),ByN(M,i));
\[ k4x = \text{dSxdt}(Sy(M,i)+B(4,1)*h*k1y+B(4,2)*h*k2y+B(4,3)*h*k3y,Sz(M,i) +B(4,1)*h*k1z+B(4,2)*h*k2z+B(4,3)*h*k3z,ByN(M,i),BzN(M,i)); \]
\[ k4y = \text{dSydt}(Sx(M,i)+B(4,1)*h*k1x+B(4,2)*h*k2x+B(4,3)*h*k3x,Sz(M,i) +B(4,1)*h*k1z+B(4,2)*h*k2z+B(4,3)*h*k3z,BxN(M,i),BzN(M,i)); \]
\[ k4z = \text{dSzdt}(Sx(M,i)+B(4,1)*h*k1x+B(4,2)*h*k2x+B(4,3)*h*k3x,Sy(M,i) +B(4,1)*h*k1y+B(4,2)*h*k2y+B(4,3)*h*k3y,BxN(M,i),ByN(M,i)); \]
\[ k5x = \text{dSxdt}(Sy(M,i)+B(5,1)*h*k1y+B(5,2)*h*k2y+B(5,3)*h*k3y +B(5,4)*h*k4y,Sz(M,i)+B(5,1)*h*k1z+B(5,2)*h*k2z+B(5,3)*h*k3z +B(5,4)*h*k4z,ByN(M,i),BzN(M,i)); \]
\[ k5y = \text{dSydt}(Sx(M,i)+B(5,1)*h*k1x+B(5,2)*h*k2x+B(5,3)*h*k3x +B(5,4)*h*k4x,Sz(M,i)+B(5,1)*h*k1z+B(5,2)*h*k2z+B(5,3)*h*k3z +B(5,4)*h*k4z,BxN(M,i),BzN(M,i)); \]
\[ k5z = \text{dSzdt}(Sx(M,i)+B(5,1)*h*k1x+B(5,2)*h*k2x+B(5,3)*h*k3x +B(5,4)*h*k4x,Sy(M,i)+B(5,1)*h*k1y+B(5,2)*h*k2y+B(5,3)*h*k3y +B(5,4)*h*k4y,BxN(M,i),ByN(M,i)); \]
\[ k6x = \text{dSxdt}(Sy(M,i)+B(6,1)*h*k1y+B(6,2)*h*k2y+B(6,3)*h*k3y +B(6,4)*h*k4y+B(6,5)*h*k5y,Sz(M,i)+B(6,1)*h*k1z+B(6,2)*h*k2z +B(6,3)*h*k3z+B(6,4)*h*k4z+B(6,5)*h*k5z,ByN(M,i),BzN(M,i)); \]
\[ k6y = \text{dSydt}(Sx(M,i)+B(6,1)*h*k1x+B(6,2)*h*k2x+B(6,3)*h*k3x +B(6,4)*h*k4x+B(6,5)*h*k5x,Sz(M,i)+B(6,1)*h*k1z+B(6,2)*h*k2z +B(6,3)*h*k3z+B(6,4)*h*k4z+B(6,5)*h*k5z,BxN(M,i),BzN(M,i)); \]
\[ k6z = \text{dSzdt}(Sx(M,i)+B(6,1)*h*k1x+B(6,2)*h*k2x+B(6,3)*h*k3x +B(6,4)*h*k4x+B(6,5)*h*k5x,Sy(M,i)+B(6,1)*h*k1y+B(6,2)*h*k2y +B(6,3)*h*k3y+B(6,4)*h*k4y+B(6,5)*h*k5y,BxN(M,i),ByN(M,i)); \]

\[ Sx(M,i+1) = Sx(M,i)+h*(CH(1)*k1x + CH(2)*k2x + CH(3)*k3x + CH(4)*k4x+CH(5)*k5x+CH(6)*k6x); \]
\[ Sy(M,i+1) = Sy(M,i)+h*(CH(1)*k1y + CH(2)*k2y + CH(3)*k3y + CH(4)*k4y+CH(5)*k5y+CH(6)*k6y); \]
\[ Sz(M,i+1) = Sz(M,i)+h*(CH(1)*k1z + CH(2)*k2z + CH(3)*k3z + CH(4)*k4z+CH(5)*k5z+CH(6)*k6z); \]

\[ [\sigma_i, \sigma_j] = 2i\varepsilon_{ijk}\sigma_k \quad \text{(A.1)} \]
\[ \{\sigma_i, \sigma_j\} = 2\delta_{ij}I \quad \text{(A.2)} \]

A.2 A2

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\[ [\sigma_i, \sigma_j] + \{\sigma_i, \sigma_j\} = \sigma_i \sigma_j - \sigma_i \sigma_j + \sigma_j \sigma_i = 2 \sigma_i \sigma_j = 2i \epsilon_{ijk} \sigma_k + 2 \delta_{ij} I \] (A.3)

\[ \rightarrow \sigma_i \sigma_j = i \epsilon_{ijk} \sigma_k + \delta_{ij} I \] (A.4)

Given:
\[ \vec{u} = (u_i, u_j, u_k), \vec{v} = (v_i, v_j, v_k) \] (A.5)

\[ (u_i v_j)(\sigma_i \sigma_j) = (u_i v_j)[i \epsilon_{ijk} \sigma_k + \delta_{ij} I] = i(\epsilon_{ijk} u_i v_j) \sigma_k + u_i v_i I = (u_i \sigma_i)(v_j \sigma_j) \] (A.6)

\[ \rightarrow (\vec{u} \cdot \hat{\sigma})(\vec{v} \cdot \hat{\sigma}) = i(\vec{u} \times \vec{v})_k \sigma_k + (\vec{u} \cdot \vec{v}) I = (\vec{u} \times \vec{v}) \cdot \sigma + (\vec{u} \cdot \vec{v}) I \] (A.7)

If \( \vec{u} = \vec{v} = \hat{n} \), then for \( n = 0, 1, 2, \ldots \):

\[ (\vec{u} \cdot \hat{\sigma})(\vec{v} \cdot \hat{\sigma}) = (\vec{u} \cdot \hat{\sigma})^2 = I \] (A.8)

\[ \rightarrow (\vec{u} \cdot \hat{\sigma})^{2n} = I, (\vec{u} \cdot \hat{\sigma})^{2n+1} = (\vec{u} \cdot \hat{\sigma}) \] (A.9)

\[ e^{i \theta \hat{\sigma} \cdot \sigma} = \sum_{n=0}^{\infty} \frac{(i \theta)^n}{n!} (\vec{u} \cdot \hat{\sigma})^n = \sum_{n=0}^{\infty} \frac{i^{2n} \theta^{2n}}{(2n)!} (\vec{u} \cdot \hat{\sigma})^{2n} + \sum_{n=0}^{\infty} \frac{i^{2n+1} \theta^{2n+1}}{(2n+1)!} (\vec{u} \cdot \hat{\sigma})^{2n+1} \]

\[ = \sum_{n=0}^{\infty} \frac{(-1)^n \theta^{2n}}{(2n)!} I + \sum_{n=0}^{\infty} \frac{i(-1)^n \theta^{2n+1}}{(2n+1)!} (\vec{u} \cdot \hat{\sigma}) = I \cos \theta + i \vec{u} \cdot \hat{\sigma} \sin \theta \] (A.10)
The expectation value of $\sigma_y$ with first order corrections to the eigenstates for $m = m'$ gives the following terms for the expressions in the large bracket of Equation 4.49

\[ m = m' = 1, m'' = \pm 1 \]

\[
e^{i\omega t} \left[ i J_q(x)(-1)^q - i J_q(x) + i y \left( J_{q'-q}(x)(-1)^{q'-q} + m'' J_{q'-q}(x) \right) \right] \]

\[ - J_{q'-q}(x)(-1)^{q'-q} - m'' J_{q'(x)} \]

\[ + i y \frac{J_q(x)(-1)^q + m'' J_q(x)}{4q'} \]

\[ - J_{q'-q}(x) + m'' J_{q'-q}(x)(-1)^{q'-q} \]

\[ + i y \frac{J_q(x)(-1)^q - J_q(x)}{4q'} \]

\[ - J_{q'-q}(x) - J_{q'-q}(x)(-1)^{q'-q} \]

\[ + i y \left( J_{q'-q}(x)(-1)^{q'-q} - J_{q'-q}(x) \right) J_q(x) \]

\[ + 2i y \left( J_{q'-q}(x)(-1)^{q'-q} J_{q'-q}(x) + J_q(x) J_{q'-q}(x)(-1)^{q'-q} \right) \]

\[ + 2i y \frac{J_q(x)(-1)^q - J_q(x)}{4q'} \]

\[ \left( J_{q'-q}(x)(-1)^{q'-q} J_{q'-q}(x) + J_q(x) J_{q'-q}(x)(-1)^{q'-q} \right) \]

Adding the terms together between the choices for all $m$'s we have:

\[ e^{i\omega t} \left[ J_{q'-q}(x)(-1)^{q'-q} J_{q'-q}(x) + J_q(x) J_{q'-q}(x)(-1)^{q'-q} \right] \]

\[ + J_{q'-q}(x)(-1)^{q'-q} J_q(x)(-1)^{q'-q} - J_{q'-q}(x) J_q(x) \]

\[ \frac{q'}{q'-q} \]

\[ + \frac{q'-q}{q'} \]

(A.11)

(A.12)
A.4 A4

The cases I ignored for the first order corrections to $\langle \sigma_y(t) \rangle$ are for $m \neq m'$, $q$ odd or even and $m = m'$, $q$ even. The expectation value is

$$
\langle \sigma_y(t) \rangle = \sum_{m, m', m''} \sum_{q, q'} \frac{1}{2} \sum \alpha^* \alpha e^{i q_0 t} e^{i (m-m') \omega_d t/2} \left[ i m J_q(x)(-1)^q - i m' J_q(x) \right] + i y \left[ \frac{m' J_{q-q}(x)(-1)^{q'-q} + m'' J_{q-q}(x)}{4(q'-q)} \right] \left[ m J_{q'}(x)(-1)^q - m'' J_{q'}(x) \right] + i y \left[ \frac{m J_q(x)(-1)^q + m'' J_q(x)}{4q'} \right] \left[ -m' J_{q-q}(x) + m'' J_{q-q}(x)(-1)^{q'-q} \right].
$$

(A.13)

For $m = m' = \pm 1$, Equation A.11 can be used again for evaluating even $q$

$$
\frac{1}{2} i y \sum_{q\text{ even}, q'} e^{i q_0 t} \left[ \frac{-J_q(x)(-1)^q J_{q-q}(x) + J_{q'}(x)J_{q-q}(x)(-1)^{q'-q}}{q'} \right] + \frac{J_{q-q}(x)(-1)^{q'-q} J_q(x)(-1)^q - J_{q-q}(x)J_q(x)}{(q'-q)}.
$$

(A.14)

Then account for negative $q$'s and looking at each $q'$ case

$$
\frac{1}{2} i y \sum_{q\geq 0, \text{ even}} \left[ e^{i q_0 t} + e^{-i q_0 t} \right] \times \left\{ \sum_{q' \text{ odd}, q-q \text{ odd}} \left[ \frac{J_q(x)J_{q-q}(x) - J_{q'}(x)J_{q-q}(x)}{q'} + \frac{J_{q-q}(x)J_q(x) - J_{q-q}(x)J_{q'}(x)}{q'-q} \right] \right\} + \sum_{q' \text{ even}, q-q \text{ even}} \left[ \frac{-J_q(x)J_{q-q}(x) + J_{q'}(x)J_{q-q}(x)}{q'} + \frac{J_{q-q}(x)J_q(x) - J_{q-q}(x)J_{q'}(x)}{q'-q} \right]
$$

(A.15)

$$
= 0.
$$

The next case is for $m \neq m'$
\[ m = 1, m' = -1, m'' = \pm 1 \]

\[
\frac{1}{2} e^{i\omega t} e^{i\omega_d t} \left[ i J_q(x)(-1)^q + i J_q(x) + i y \frac{[J_q(x)(-1)^q - m'' J_q(x)]}{4(q' - q)} \right] \]

\[
+ i y \frac{J_q(x)(-1)^q + m'' J_q(x)}{4q'} \left[ J_q(x)(-1)^q - J_q(x) \right] \]

\[
+ \frac{1}{2} e^{i\omega t} e^{i\omega_d t} \left[ i J_q(x)(-1)^q + i J_q(x) + i y \frac{[J_q(x)(-1)^q - m'' J_q(x)]}{4(q' - q)} \right] \]

\[
+ i y \frac{J_q(x)(-1)^q + J_q(x)}{4q'} \left[ J_q(x) - J_q(x)(-1)^q \right] \]

\[
= \frac{1}{2} e^{i\omega t} e^{i\omega_d t} \left[ i J_q(x)(-1)^q + i J_q(x) + 2i y \frac{J_q(x)(-1)^q - J_q(x)(-1)^q + J_q(x)(-1)^q}{4(q' - q)} \right] \]

\[
+ 2i y \frac{J_q(x)(-1)^q J_q(x)(-1)^q}{4q'} \]

\[ m = -1, m' = 1, m'' = \pm 1 \]

\[
\frac{1}{2} e^{i\omega t} e^{-i\omega_d t} \left[ -i J_q(x)(-1)^q - i J_q(x) + i y \frac{[J_q(x)(-1)^q - m'' J_q(x)]}{4(q' - q)} \right] \]

\[
+ i y \frac{[J_q(x)(-1)^q + m'' J_q(x)]}{4q'} \left[ J_q(x)(-1)^q - J_q(x)(-1)^q \right] \]

\[
= \frac{1}{2} e^{i\omega t} e^{-i\omega_d t} \left[ -i J_q(x)(-1)^q - i J_q(x) + i y \frac{[J_q(x)(-1)^q - m'' J_q(x)]}{4(q' - q)} \right] \]

\[
+ i y \frac{J_q(x)(-1)^q + J_q(x)}{4q'} \left[ J_q(x) + J_q(x)(-1)^q \right] \]

\[
+ \frac{1}{2} e^{i\omega t} e^{-i\omega_d t} \left[ i y \frac{J_q(x)(-1)^q - J_q(x)}{4(q' - q)} \right] \]

\[
+ i y \frac{J_q(x)(-1)^q - J_q(x)}{4q'} \left[ J_q(x) - J_q(x)(-1)^q \right] \]

\[
= \frac{1}{2} e^{i\omega t} e^{-i\omega_d t} \left[ -i J_q(x)(-1)^q - i J_q(x) + 2i y \frac{J_q(x)(-1)^q - J_q(x)(-1)^q + J_q(x)(-1)^q}{4(q' - q)} \right] \]

\[
+ 2i y \frac{J_q(x)(-1)^q J_q(x)(-1)^q}{4q'} \]

The expectation value for \( m \neq m' \) is

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$$\langle \sigma_y(t) \rangle |_{m \neq m'} = \sum_{q,q'} e^{iq\omega_{a}t} \left\{ e^{i\omega_{a}t} \left[ \frac{1}{2} i J_q(x)(-1)^q + \frac{1}{2} i J_q(x) \right] \\
+ i y \frac{-J_{q'-q}(x)(-1)^{q'-q} J_{q'}(x)(-1)^q - J_{q'-q}(x) J_{q'}(x)}{4(q'-q)} \\
+ i y \frac{J_{q'}(x)(-1)^q J_{q'-q}(x) + J_{q'}(x) J_{q'-q}(x)(-1)^{q'-q}}{4q'} \\
+ e^{-i\omega_{a}t} \left[ -\frac{1}{2} i J_q(x)(-1)^q - \frac{1}{2} i J_q(x) \right] \\
+ i y \frac{-J_{q'-q}(x)(-1)^{q'-q} J_{q'}(x)(-1)^q - J_{q'-q}(x) J_{q'}(x)}{4(q'-q)} \\
+ i y \frac{J_{q'}(x)(-1)^q J_{q'-q}(x) + J_{q'}(x) J_{q'-q}(x)(-1)^{q'-q}}{4q'} \right\}$$

(A.17)

$$= \sum_{q,q'} e^{iq\omega_{a}t} \left\{ e^{i\omega_{a}t} \left[ \frac{1}{2} i J_q(x)(-1)^q + \frac{1}{2} i J_q(x) \right] \\
+ i y \left[ e^{i\omega_{a}t} + e^{-i\omega_{a}t} \right] \left[ \frac{-J_{q'-q}(x)(-1)^{q'-q} J_{q'}(x)(-1)^q - J_{q'-q}(x) J_{q'}(x)}{4(q'-q)} \\
+ \frac{J_{q'}(x)(-1)^q J_{q'-q}(x) + J_{q'}(x) J_{q'-q}(x)(-1)^{q'-q}}{4q'} \right] \right\}$$

$$= \sum_{q,q'} e^{iq\omega_{a}t} \left\{ i\sin\omega_{a}t \left[ i J_q(x)(-1)^q + i J_q(x) \right] \\
+ 2i y \cos\omega_{a}t \left[ \frac{-J_{q'-q}(x)(-1)^{q'-q} J_{q'}(x)(-1)^q - J_{q'-q}(x) J_{q'}(x)}{4(q'-q)} \\
+ \frac{J_{q'}(x)(-1)^q J_{q'-q}(x) + J_{q'}(x) J_{q'-q}(x)(-1)^{q'-q}}{4q'} \right] \right\}.$$
The first term is the zeroth order term from [Gol94]. For all the first order terms, it is clear where some of them cancel each other like in the numerators of the \( q' \) sums for \( q \) odd. For even \( q \) and even \( q' \), the denominators will be even and given opposite signs between the two terms, they will cancel each other out. The first order results in Equation A.18 become

\[
<\sigma_y(t)\rangle_{m\neq m'} = \sum_{q \text{ even}} i \sin \omega_d t e^{i q \omega t} \left[ iJ_q(x) + iJ_q(x) \frac{-J_{q-q}(x)J_{q}(x)}{2(q'-q)} + \frac{J_q(x)J_{q-q}(x)}{2q'} \right] + \sum_{q \text{ odd}} \left\{ e^{i q \omega t} i y \cos \omega_d t \sum_{q' \text{ even}} \left[ \frac{J_{q-q}(x)J_q(x) - J_{q-q}(x)J_q(x)}{2(q'-q)} \right. \right. \\
+ \left. \left. \frac{-J_q(x)J_{q-q}(x) - J_q(x)J_{q-q}(x)}{2q'} \right] + \sum_{q' \text{ odd}} \left[ \frac{J_{q-q}(x)J_q(x) - J_{q-q}(x)J_q(x)}{2(q'-q)} \right. \right. \\
+ \left. \left. \frac{-J_q(x)J_{q-q}(x) - J_q(x)J_{q-q}(x)}{2q'} \right] \right\} \right. \\
+ \sum_{q \text{ even}} -2 \sin \omega_d t e^{i q \omega t} J_q(x) \sum_{q' \text{ odd}} \left[ \frac{-J_{q-q}(x)J_q(x)}{(q'-q)} + \frac{-J_q(x)J_{q-q}(x)}{q'} \right] \\
(A.18)
\]

where the last term sum over \( q \) cannot have \( q = 0 \) or all terms for the sum over \( q' \) will vanish. This will actually be the case for all terms since no matter what \( q' - q \) is odd. Some terms for \( q = \pm 2 \) and \( q' = \pm 1 \) are
Thus, all terms have vanished.

**A.5**

The expectation value of $\sigma_z$ with first order corrections to the eigenstates has the following selection rules
\[ m = m' = 1, m'' = \pm 1 \]
\[ e^{iq\omega t} \left[ y \left[ J_{q'-q}(x)(-1)^{q'-q} + m'' J_{q'-q}(x) \right] \left[ J_{q'}(x)(-1)^{q'} + m'' J_{q'}(x) \right] \right. \]
\[ + y \left[ J_{q'}(x)(-1)^{q'} + m'' J_{q'}(x) \right] \left[ J_{q'-q}(x)(-1)^{q'-q} \right] \]
\[ = e^{iq\omega t} \left[ y \left[ J_{q'-q}(x)(-1)^{q'-q} + J_{q'-q}(x) \right] \left[ J_{q'}(x)(-1)^{q'} + J_{q'}(x) \right] \right. \]
\[ + y \left[ J_{q'}(x)(-1)^{q'} + J_{q'}(x) \right] \left[ J_{q'-q}(x)(-1)^{q'-q} \right] \]
\[ = e^{iq\omega t} \left[ 2y \frac{J_{q'-q}(x)(-1)^{q'-q} J_{q'}(x)(-1)^{q'} + J_{q'-q}(x) J_{q'}(x)}{4(q'-q)} \right. \]
\[ + 2y \frac{J_{q'}(x)(-1)^{q'} J_{q'-q}(x) + J_{q'}(x) J_{q'-q}(x)(-1)^{q'-q}}{4q'} \right]. \]  

\( (A.21) \)

\[ m = m' = -1, m'' = \pm 1 \]
\[ e^{iq\omega t} \left[ y \left[ -J_{q'-q}(x)(-1)^{q'-q} + m'' J_{q'-q}(x) \right] \left[ -J_{q'}(x)(-1)^{q'} + m'' J_{q'}(x) \right] \right. \]
\[ + y \left[ -J_{q'}(x)(-1)^{q'} + m'' J_{q'}(x) \right] \left[ -J_{q'-q}(x)(-1)^{q'-q} \right] \]
\[ = e^{iq\omega t} \left[ y \left[ -J_{q'-q}(x)(-1)^{q'-q} + J_{q'-q}(x) \right] \left[ -J_{q'}(x)(-1)^{q'} + J_{q'}(x) \right] \right. \]
\[ + y \left[ -J_{q'}(x)(-1)^{q'} + J_{q'}(x) \right] \left[ -J_{q'-q}(x)(-1)^{q'-q} \right] \]
\[ = e^{iq\omega t} \left[ 2y \frac{-J_{q'-q}(x)(-1)^{q'-q} J_{q'}(x)(-1)^{q'} + J_{q'-q}(x) J_{q'}(x)}{4(q'-q)} \right. \]
\[ + 2y \frac{-J_{q'}(x)(-1)^{q'} J_{q'-q}(x) + J_{q'}(x) J_{q'-q}(x)(-1)^{q'-q}}{4q'} \right]. \]  

A.6  A6

Given the following relation (a proof can be found in Appendix A1)
where $S$ is the field for time $\tau$ and the $-\omega_z$ for a time $\tau$, the time evolution operator becomes

$$U_{\pm}(2\tau) = e^{-iH_{\pm}\tau} e^{-iH_z \tau}$$

$$= e^{-\tau/2\tau_0} \left( e^{-i\omega_z \tau} - i \epsilon \sin \omega_z \tau / \omega_z \tau \right) e^{-\tau/2\tau_0} \left( e^{i\omega_z \tau} - i \epsilon \sin \omega_z \tau / \omega_z \tau \right)$$

$$= e^{-\tau/\tau_0} \left( 1 - e^2 \sin^2 \omega_z \tau \right) e^{i\omega_z \tau} \left( -2i \epsilon e^{-i\omega_z \tau} \sin \omega_z \tau \right)$$

$$= e^{-\tau/\tau_0} \left( 1 - 2i \epsilon e^{i\omega_z \tau} \sin \omega_z \tau \right) + e^{-\tau/\tau_0} \left( 0 O(\epsilon^2) 0 \right).$$

I will ignore the small $\epsilon^2 << 1$ terms. Equation 5.10 can be written as

$$U_{\pm}(2\tau) = e^{-\tau/\tau_0}(1 + b \sigma_i),$$

where $b = -2i \epsilon \sin \omega_z \tau$ and $\sigma_i$ is

$$\sigma_i = \begin{pmatrix} 0 & e^{i\omega_z \tau} \\ e^{-i\omega_z \tau} & 0 \end{pmatrix}.$$
\[ M = I + b \sigma_1. \] (A.28)

Then using binomial theorem as shown in the Physics Reports Appendix [Gol94], the matrix M to power \( n \) can be written as

\[ M^n = \frac{1}{2}((1+b)^n + (1-b)^n) + \sigma_1 \frac{1}{2}[(1+b)^n - (1-b)^n], \] (A.29)

so that Equation 5.11 to the power \( n \) can be written as

\[ [U_{\pm}(2\tau)]^n \equiv U_n = \frac{1}{2}[(1+b)^n + (1-b)^n] + \frac{1}{2} \sigma_1[(1+b)^n - (1-b)^n]e^{-n\tau/\tau_0}. \] (A.30)

Now for the calculation of terms \((1 \pm b)^n\), I’ll expand b, define \( T = 2\tau n \) the total measurement time and take advantage of the approximation: \((1 + x/n)^n \approx e^x\) for \( n \gg 1\)

\[ (1 \pm b)^n = \left[ 1 \mp 2iP_3\alpha'\sin(\omega_z T/\omega_z \tau) \right]^n \]

\[ = \left[ 1 \mp 2iP_3\alpha'\sin(\omega_z T/\omega_z \tau) \frac{T}{2n} \right]^n \approx e^{\mp iP_3\alpha'T\sin(\omega_z T/\omega_z \tau)} \equiv e^{\mp i\alpha}, \] (A.31)

where \( \alpha = ib T/\tau \). Now \( U_n \) becomes

\[ U_n = \frac{1}{2} \left[ e^{-i\alpha} + e^{i\alpha} \right] + \frac{1}{2} \sigma_1 \left[ e^{i\alpha} - e^{-i\alpha} \right] e^{-T/2\tau_0} \]

\[ = \frac{1}{2} e^{-T/2\tau_0} \left( \begin{array}{cc} F_+ & F_- e^{i\omega_z \tau} \\ F_- e^{-i\omega_z \tau} & F_+ \end{array} \right), \] (A.32)

where \( F_\pm = \left[ e^{-i\alpha} \pm e^{i\alpha} \right] \). For the final step of this derivation, we start with the first pulse of the modulation which is to apply a \( -\omega_z \) pulse for time \( \tau/2 \). \( U_{\pm}(\tau/2) \) is trivial to find at this point and the whole modulation sequence will give

\[ U_{\pm}(T) = U_n e^{-iH_{\omega_z} \tau/2} \]

\[ = \left[ \frac{1}{2} \left[ e^{-i\alpha} + e^{i\alpha} \right] + \frac{1}{2} \sigma_1 \left[ e^{i\alpha} - e^{-i\alpha} \right] \right] e^{-T/2\tau_0} \] (A.33)

\[ = \frac{1}{2} e^{-T/2\tau_0} \left( \begin{array}{cc} F_+ & F_- e^{i\omega_z \tau/2} \\ F_- e^{-i\omega_z \tau/2} & F_+ \end{array} \right) \left( \begin{array}{cc} e^{i\omega_z \tau/2} & 0 \\ 0 & e^{-\omega_z \tau/2} \end{array} \right) \]

\[ = \frac{1}{2} e^{-T/2\tau_0} \left( \begin{array}{cc} F_+ e^{i\omega_z \tau/2} & F_- e^{-i\omega_z \tau/2} \\ F_- e^{-i\omega_z \tau/2} & F_+ e^{i\omega_z \tau/2} \end{array} \right). \] (A.34)

Now we have what we need to find an expectation value. For polarized neutrons initially pointing along the \( \pm x \)-axis, the time independent wave function at \( t = 0 \) is

\[ \psi_\pm(0) = \frac{1}{\sqrt{2}} \left( \begin{array}{c} 1 \\ \pm 1 \end{array} \right). \] (A.35)
The total time dependent wave function is
\[ \psi_\pm(T) = U_{tot}(T)\psi(0) = \frac{1}{2\sqrt{2}} (F_+ \pm F_-) \left( e^{i\omega_z \tau/2} \pm e^{-i\omega_z \tau/2} \right). \] (A.36)

And the expectation value of \( \sigma_x(t) \) is
\[
< \sigma_x(t) > = \psi_\pm^*(T)\sigma_x\psi_\pm(T)
= \frac{e^{-T/2\tau_0}}{2\sqrt{2}} (F_+ \pm F_-) \left( e^{-i\omega_z \tau/2} \pm e^{i\omega_z \tau/2} \right) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}
\times \left( e^{i\omega_z \tau/2} \right) \frac{e^{-T/2\tau_0}}{2\sqrt{2}} (F_+ \pm F_-)
= \left[ \frac{e^{-T/2\tau_0}}{2\sqrt{2}} \right]^2 |F_+ \pm F_-|^2 \left( \pm e^{-i\omega_z \tau} \pm e^{i\omega_z \tau} \right)
= \pm \frac{e^{-T/\tau_0}}{4} |F_+ \pm F_-|^2 \cos \omega_z \tau
= \pm \frac{e^{-T/\tau_0}}{4} e^{\pm 2P_3 T/\tau_3} \sin \omega_z \tau \cos \omega_z \tau. \] (A.37)

As can be seen, the expectation value does not depend on the pseudomagnetic field strength \( A \) meaning the modulations offset its affect.