Investigation of the Higher Order Zeeman Effect

By

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TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

CHAPTER 1

The Higher Order Zeeman Effect

1.1 OVERVIEW

In this chapter the Zeeman Effect is introduced, and the motivation, direct applications, and the higher order Zeeman Effect is discussed. The main focus of this chapter is to show the effect of the quadratic Zeeman Effect, and show how using the relativistic magnetic dipole operator in conjunction with the relativistic corrections to $^3He^+$ yields a cubic Zeeman Effect. The effects of both the quadratic and cubic corrections are discussed in great detail, and the impact of the effect on high precision measurements is displayed for various magnetic field strengths.

Sec. 1.2 starts with the history of the Zeeman effect, its origins and discovery. Afterwards the motivation for the project in Sec. 1.3 is discussed. Here, some current experiments in the field such as the $g-2$ experiment conducted at the Max Planck Institute as well as applications to high-precision magnetometry are highlighted. Some additional applications such as the shift in spectral lines of neutron stars and magnetic white dwarfs are introduced as well. In Sec. 1.4, the ordinary Zeeman effect and quadratic Zeeman effect are derived using the canonical momentum. Their respective theories are introduced and applications to atomic systems such as $^3He^+$ are discussed. Moving towards higher order systems, the cubic Zeeman effect is introduced. Starting with the effects that contribute to the cubic Zeeman effect such as the relativistic magnetic dipole operator in Sec. 1.5.1 and the quadratic Zeeman effect, the relativistic correction to $^3He^+$ is derived and shown in Sec. 1.5.2. these effects are combined to yield a B^3 contribution to the energy splitting within the presence of an external magnetic field. Afterwards, Sec. 1.6 discusses the results of the calculation and its applications.

1.2 HISTORY

The Zeeman effect was first introduced by Pieter Zeeman, who discovered in 1896 that in the presence of a static magnetic field, spectral lines could be split into many components. After the discovery of quantum mechanics, the behaviour was found to be described as a perturbation of the Hamiltonian using the magnetic moment of the atom and the magnetic field.

Since it's discovery, the Zeeman effect has played a large role in the field of atomic physics and magnetometry, which is the study of the intensity of magnetic field across space and time. There have been several calculations to include the relativistic corrections [32, 33], field inhomogeneities, and quadratic effects in hydrogenic systems [20]. However, little is known about its behavior in helium atoms such as $^3\mathrm{He}^+$ and $^3\mathrm{He}$, which is of key interest in magnetometry and the muon magnetic moment anomaly $(\mu_g - 2)$, for which there is a 5.0 σ discrepancy [9] with the standard model prediction.

1.3 MOTIVATION

1.3.1 The $g-2$ experiment

The Dirac equation is a very successful and well studied equation in quantum mechanics. Its success comes from its ability to predict 2 important phenomena; the existence of antimatter and the magnetic dipole moment of the electron. The Dirac equation predicts that the magnetic dipole of the electron should be twice that of the classical prediction. This result is expressed in terms of the g-factor which the Dirac equation predicts is equal to 2. While the Dirac prediction is much closer to experimental findings, there is still a difference between the experimentally measured value of g and the equations prediction. This is called the $g-2$ anomaly. The anomaly is represented by

$$a = \frac{g-2}{2}\ . \tag{1.1}$$

The ~~discrepancy~~ of g is caused by higher-order contributions from quantum field theory and to this day is yet to be properly explained.

$$a_\mu^{\mathrm{SM}} = a_\mu^{\mathrm{QED}} + a_\mu^{\mathrm{EW}} + a_\mu^{\mathrm{hadron}} \tag{1.2}$$

The first two terms can be derived from first principles, but the hadronic term cannot be calculated precisely on its own and is estimated from experimental results. The effort to measure the muon magnetic moment precisely is an active area of research. The work presented in this thesis aids in the investigation of the $g-2$ anomaly by providing corrections to the Zeeman splitting in $^3He^+$, the element used in the magnetometry experiment to measure the anomaly. Accounting for higher order corrections to the Zeeman effect may help consolidate the discrepancy between theory and experiment and help researchers further understand the muon magnetic moment and its impact on muonic systems.

1.3.2 High-precision magnetometry

1.3.3 Connection to Atomic Physics

1.4 THE ZEEMAN EFFECT

When an atom is placed in an external magnetic field, its energy levels are shifted. The shifting of energy levels is known as the Zeeman effect. The effect is derived from the Schrodinger equation and the canonical momentum. The canonical momentum is a conserved quantity that describes a moving charged particle. It can be written as

$$\vec{p} = m\vec{v} + e\vec{A}\ . \tag{1.3}$$

Where $m\vec{v}$ is the classical definition of the momentum, and $e\vec{A}$ is the extension from electrodynamics that accounts for the impact of an external magnetic field on a charged particle. This term is required in order to ensure that the conservation of momentum holds true, since charged particles subject to an external magnetic field travel in a circular path dependant on the direction of the field.

The canonical momentum then is also written in replacement to the typical momentum operator in quantum mechanics, giving the canonical momentum operator

$$\hat{p}_{\text{canonical}} = i\hbar\vec{\nabla} + e\hat{A}\ . \tag{1.4}$$

Where $\hat{A}$ is the vector potential operator. For an external magnetic field of strength B pointing in the $\hat{k}$ direction the operator becomes

$$\hat{A} = \frac{B}{2}\left(y\hat{i} - x\hat{j}\right)\ . \tag{1.5}$$

Substituting this in for the vector potential operator in the canonical momentum and placing it into the Hamiltonian equation one gets

$$\hat{H} = \frac{\left(i\hbar\vec{\nabla} + \frac{Be}{2}\left(y\hat{i} - x\hat{j}\right)\right)^2}{2m_e} - \frac{Ze^2}{4\pi\epsilon_0\vec{r}}\ . \tag{1.6}$$

Which when expanded gives

$$\hat{H} = \frac{-\hbar^2\nabla^2}{2m} - \frac{i\hbar eB}{4mc}\vec{\nabla}\cdot\left[y\hat{i} - x\hat{j}\right] - \frac{i\hbar eB}{4mc}\left[y\hat{i} - x\hat{j}\right]\cdot\vec{\nabla} + \frac{e^2B^2}{8mc}\left(x^2 + y^2\right) - \frac{Ze^2}{4\pi\epsilon_0 r}\ . \tag{1.7}$$

This equation is crucial for incorporating elecromagnetic effects into the Hamiltonian. The first term in the expanded Hamiltonian is the standard operator. The first term and last term of the equation can be combined to write the ordinary Hamiltonian

$$\hat{H} = \hat{H}_{\text{Standard}} - \frac{i\hbar eB}{4mc}\vec{\nabla} \cdot \left[y\hat{\imath} - x\hat{\jmath}\right] - \frac{i\hbar eB}{4mc}\left[y\hat{\imath} - x\hat{\jmath}\right] \cdot \vec{\nabla} + \frac{e^2B^2}{8mc}\left(x^2 + y^2\right) \ . \tag{1.8}$$

When $\vec{\nabla} \cdot \hat{A} = 0$, it is permitted to replace $\nabla \cdot \hat{A}$ with $\hat{A} \cdot \vec{\nabla}$ [28]. Performing the dot product in the next term gives

$$\hat{H} = \hat{H}_{\text{Standard}} - \frac{i\hbar eB}{2mc}\left[y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}\right] + \frac{e^2B^2}{8mc}\left(x^2 + y^2\right) \ . \tag{1.9}$$

This term is analgous to the orbital angular momentum operator in the $\hat{k}$ direction

$$L_z = xp_y - yp_x = i\hbar\left[y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}\right] \ . \tag{1.10}$$

Substituting this into the expression for the total Hamiltonian

$$\hat{H} = \hat{H}_{\text{Standard}} + \frac{eB}{2mc}L_z + \frac{e^2B^2}{8mc}\left(x^2 + y^2\right) \ . \tag{1.11}$$

The middle term is the angular magnetic moment of the system, and the final term containing a B^2 is known as the quadratic Zeeman effect $\hat{H}_Z^{(2)}$. The orbital angular magnetic moment is [12]

$$\vec{\mu}_\ell = \frac{e}{2mc}\vec{L} \ . \tag{1.12}$$

Thus the Hamiltonian for a system subject to an external magnetic field is

$$\hat{H} = \hat{H}_{\text{Standard}} + \hat{H}_{\vec{\mu}_\ell} + \hat{H}_Z^{(2)} \ . \tag{1.13}$$

Since the magnetic field in question is considered to be in the positive $\hat{k}$ direction, the linear Zeeman effect term is written in terms of the orbital magnetic moment

$$\hat{H}_Z^{(1)} = \vec{\mu}_\ell \cdot \vec{B} \ . \tag{1.14}$$

Accounting for the intrinsic spin of the electron, an additional term can be added to the Hamiltonian called the spin interaction [28]

$$\hat{H}_{\text{Spin}} = -g_s \frac{eB}{2mc} \vec{S} \ . \tag{1.15}$$

Where $\vec{S}$ is the spin angular momentum operator. This expression is defined as the spin magnetic moment $\vec{\mu}_s$, and contains the Larmor frequency $\omega = \frac{eB}{2m}$ [21].

$$\vec{\mu}_s = g_s \frac{e}{2mc} \vec{S} \ . \tag{1.16}$$

Here, g_s is the electron g-factor. The spin magnetic moment and the angular magnetic moment both scale linearly in B. The two effects are combined into what is known as the linear Zeeman effect.

$$\hat{H}_Z = -\left(\vec{\mu}_\ell + \vec{\mu}_s\right) \cdot \vec{B} \ . \tag{1.17}$$

The linear Zeeman effect has the following eigen energy solutions

$$E_{n,m_s,m_\ell} = -\frac{E_0}{n^2} + \mu_B B(m_\ell + 2m_s) \ . \tag{1.18}$$

So it is seen that depending on the magnetic quantum number, the energy levels split apart. Their corresponding new energies depend on this magnetic quantum number as well as the principle quantum number n, and scale linearly with magnetic field strength B. This is shown effectively in figure. 1.4.1a.

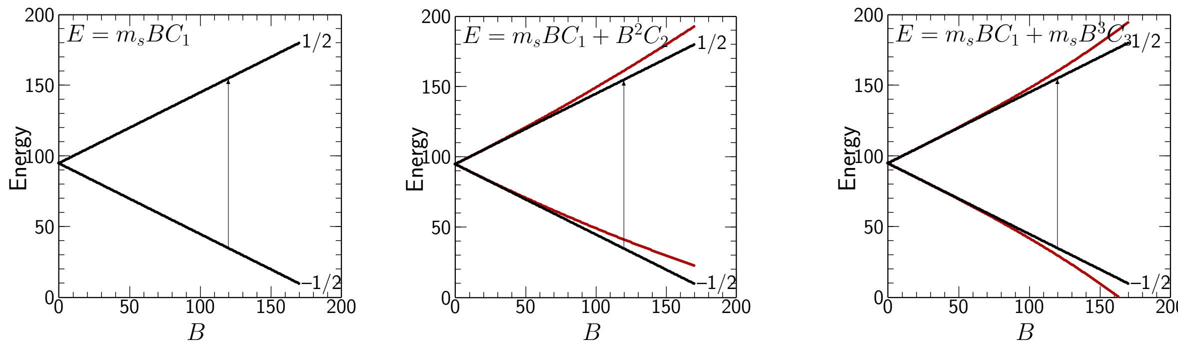
The B^2 term is the quadratic Zeeman effect and is written on its own as

$$\hat{H}_Z = \frac{B^2 e^2}{8m_e}(x^2 + y^2) \ . \tag{1.19}$$

Using $x^2 + y^2 = r^2 - z^2 = \frac{2}{3} r^2 \left[P_0(\cos\theta) - P_2(\cos\theta)\right]$ where $P_2(\cos\theta) = \frac{1}{2}\left(3\cos^2\theta - 1\right)$

and $P_0(\cos\theta) = 1$ are Legendre polynomials,

$$\hat{H}_Z = \frac{B^2 e^2}{12 m_e} r^2 (P_0(\cos\theta) - P_2(\cos\theta)) \ . \tag{1.20}$$



(a) The ordinary Zeeman effect

(b) The quadratic Zeeman effect

(c) The cubic Zeeman effect

Fig. 1.4.1: The Zeeman effect energy splitting for each order

The total Hamiltonian including the quadratic Zeeman perturbation is then

$$\hat{H} = -\frac{\hbar^2}{2m_e}\nabla^2 - \frac{Ze^2}{4\pi\epsilon_0 r} + \frac{B^2 e^2}{12 m_e} r^2 (P_0(\cos\theta) - P_2(\cos\theta)) \ . \tag{1.21}$$

Where the quadratic Zeeman term is treated as a perturbation. Using the ground state wavefunction of hydrogen for $Z = 2$ for the $^3He^+$ atom, the perturbation equation then reads

$$\left(-\frac{\hbar^2}{2m_e}\nabla^2 - \frac{Ze^2}{4\pi\epsilon_0 r} - E^{(0)}\right)|\psi^{(1)}\rangle = \left(\frac{B^2 e^2}{12 m_e} r^2 - E^{(1)}\right)\frac{Z^{\frac{3}{2}} e^{-Zr}}{\sqrt{\pi}} \ . \tag{1.22}$$

Where the $P_2(\cos\theta)$ term is zero since the problem involves spherically symmetric S states[1]. This perturbation equation can be solved using the method of Frobenius, where the form of $|\psi^{(1)}\rangle$ is assumed to be of a power series.

$$|\psi^{(1)}\rangle = \sum_{j=0}^{\infty} Z^{\frac{3}{2}} a_j r^j e^{-Zr} \tag{1.23}$$

[1]This can be proven by performing the necessary integrals with the $P_2(\cos\theta)$ term included. The result is that the $P_2(\cos\theta)$ integral is 0

Inserting $|\psi^{(1)}\rangle$ into the perturbation equation the expression reads

$$\left(-\frac{\hbar^2}{2m_e}\nabla^2 - \frac{Ze^2}{4\pi\epsilon_0 r} - E^{(0)}\right)\sum_{j=0}^{\infty} a_j r^j e^{-Zr} = \left(\frac{B^2e^2}{12m_e}r^2 - E^{(1)}\right)\frac{e^{-Zr}}{\sqrt{\pi}}\ . \tag{1.24}$$

Performing the differentiation followed by a shift of summation indices the expression simplifies to

$$\sum_{j=0}^{\infty}\left[Z(j-1)a_{j-1} - \frac{j(j+1)}{2}a_j\right]r^{j-2} = -\left(\frac{B^2e^2}{12m_e}r^2 - E^{(1)}\right)\frac{1}{\sqrt{\pi}}\ . \tag{1.25}$$

Using equation (??), $E^{(1)}$ is found to be

$$E^{(1)} = \frac{1}{4Z^2}\gamma^2\ . \tag{1.26}$$

Where $\gamma^2 \equiv \frac{B^2e^2}{m}$. The final expression before solving the recursion relation in the method of Frobenius yields

$$\sum_{j=0}^{\infty}\left[Z(j-1)a_{j-1} - \frac{j(j+1)}{2}a_j\right]r^{j-2} = -\frac{1}{12}\gamma^2\left(r^2 + \frac{3}{Z^2}\right)\frac{1}{\sqrt{\pi}}\ . \tag{1.27}$$

Grouping the powers of r from the LHS and the RHS of the equation produces a set of recursive relations that need to be solved. After substituting the correct integers for j for each equation it is seen that there are only two instances when the series terms are non-zero. These terms are for $j = 2$ and $j = 3$. All other terms in the series are zero and thus non-contributing. The solution for $|\psi^{(1)}\rangle$ is thus

$$|\psi^{(1)}\rangle = \sum_{j=0}^{\infty} a_j r^j e^{-Zr} = a_0 e^{-Zr} + a_2 r^2 e^{-Zr} + a_3 r^3 e^{-Zr} \tag{1.28}$$

Plugging in the found values for a_2 and a_3 yield

$$|\psi^{(1)}\rangle = \sum_{j=0}^{\infty} a_j r^j e^{-Zr} = a_0 e^{-Zr} - \frac{1}{12}\gamma^2\frac{1}{Z^2\sqrt{\pi}}r^2 e^{-Zr} - \frac{1}{36Z\sqrt{\pi}}\gamma^2 r^3 e^{-Zr}\ . \tag{1.29}$$

Currently, a_0 is still undetermined. It is found by imposing the orthogonality condition between $|\psi^{(0)}\rangle$ and $|\psi^{(1)}\rangle$

$$\langle\psi^{(0)}|\psi^{(1)}\rangle = 0\ . \tag{1.30}$$

~~This orthogonality relation is a choice, and it not required by any law or rule. It is necessary in order to compute a_0 and is only allowed to be chosen due to the nature of the perturbation equation. It exploits the use of the Hermitian property of the Hamiltonian that allows the operator to act to the left instead of the right. Multiplying through the original perturbation equation given in (1.21) ensures that $\left(\hat{H} - E^{(0)}\right)$ is zero, implying that any quantity can be can be added to $|\psi^{(1)}\rangle$ and the equation still holds true~~. Thus, we can add some amount to $|\psi^{(1)}\rangle$ to ensure it is orthogonal without breaking the equality. ~~This is a subtle trick, but one that is necessary to compute the full perturbed wavefunction~~[2]. The a_0 coefficient can thus be determined by calculating the integral

$$\langle\psi^{(0)}|\psi^{(1)}\rangle = \int_0^\infty \int_0^\pi \int_0^{2\pi} r^2 \sin\theta \left(a_0 - \frac{1}{12}\gamma^2 \frac{1}{\sqrt{\pi}} \left[\frac{1}{Z^2} r^2 + \frac{1}{3Z} r^3\right]\right) \frac{Z^{\frac{3}{2}} e^{-2Zr}}{\sqrt{\pi}} = 0\ . \tag{1.31}$$

And so a_0 is found to be

$$a_0 = \frac{11}{2Z^4\sqrt{\pi}} \frac{1}{12}\gamma^2\ . \tag{1.32}$$

Thus, the full first order correction to the ground state hydrogenic wavefunction subject to an external magnetic field is

$$|\psi^{(1)}\rangle = \frac{1}{12}\gamma^2 \frac{1}{\sqrt{\pi}} \left[\frac{11}{2Z^4} - \frac{1}{Z^2} r^2 - \frac{1}{3Z} r^3\right] e^{-Zr}\ . \tag{1.33}$$

[2]Further explanation of the Hermitian operator rule as well as imposing the orthogonality condition is shown in Appendix .**??**

1.5 THE CUBIC ZEEMAN EFFECT

The following section discusses the main focus of this thesis, the Cubic Zeeman effect. While the linear Zeeman affect as well as the quadratic Zeeman effect have been studied for hydrogenic systems, little is known about any higher order contributions. This section investigates the combination of the magnetic dipole moment operator and and the quadratic Zeeman effect to determine the relativistic effects of $^3He^+$ that when applied, reveal a contribution to the energy shift that is dependant on the cube of the magnetic field strength.

The section starts out by first introducing the relativistic magnetic dipole moment operator (Q_{M1}) and discusses its properties and significance to the Zeeman effect. Sec. 1.5.2 discusses the combination of the relativistic magnetic dipole moment operator with the quadratic Zeeman effect discussed in Sec .1.4 to calculate the relativistic corrections to $^3He^+$. Accounting for both interactions gives a correction to the energy splitting of $^3He^+$ dependant on B^3.

1.5.1 The relativistic magnetic dipole moment operator

The relativistic magnetic dipole moment operator represents the interaction of a magnetic dipole moment with an external magnetic field. It is described via the following relation

$$Q_{M1} = \mu_B \left(1 - \frac{2p^2}{3m^2c^2} + \frac{Ze^2}{12\pi\epsilon_0 mc^2 r}\right) \vec{\sigma} \cdot \vec{B} \tag{1.34}$$

Where μ_B is the Bohr magneton

$$\mu_B = \frac{e\hbar}{2mc} \tag{1.35}$$

The second term in the brackets of the relativistic magnetic dipole moment operator accounts for the relativistic correction to the kinetic energy of the electron, and the third term is the potential energy due to the Coulomb interaction between the electron and the nucleus. The first term corresponds to the ordinary Zeeman Effect, which does not contribute to the sum over states due to orthogonality.

The ordinary Zeeman effect contributes to Q_{M1} in $^3He^+$ because it has non-zero spin due to the missing electron. For systems such as ^3He, the ordinary Zeeman effect ~~will~~ not contribute. ~~The expression can be simplified in order to make the perturbation being applied to the hydrogenic wavefunction clearer.~~ Starting with the original expression

$$Q_{M1} = \mu_B \left(1 - \frac{2p^2}{3m^2c^2} + \frac{Ze^2}{12\pi\epsilon_0 mc^2 r} \right) \vec{\sigma} \cdot \vec{B} \ , \tag{1.36}$$

the first term can be pulled out of the expression, and the p^2 term can be written to fit the form of the Hamiltonian

$$Q_{M1} = \mu_B \vec{\sigma} \cdot \vec{B} + \frac{\mu_B}{3mc^2} \left(\frac{-4p^2}{2m} + \frac{Ze^2}{4\pi\epsilon_0 r} \right) \vec{\sigma} \cdot \vec{B} \ . \tag{1.37}$$

Subsituting in the Hamiltonian $\hat{H} = \frac{p^2}{2m} - \frac{Ze^2}{4\pi\epsilon_0 r} \longrightarrow \frac{p^2}{2m} = \hat{H} + \frac{Ze^2}{4\pi\epsilon_0 r}$ the Q_{M1} operator becomes

$$Q_{M1} = \mu_B \vec{\sigma} \cdot \vec{B} + \frac{\mu_B}{3mc^2} \left(-4\hat{H} - \frac{4Ze^2}{4\pi\epsilon_0 r} + \frac{Ze^2}{4\pi\epsilon_0 r} \right) \vec{\sigma} \cdot \vec{B} \ . \tag{1.38}$$

Simplifying the expression into 3 terms

$$Q_{M1} = \mu_B \vec{\sigma} \cdot \vec{B} + \frac{4}{3} \frac{\mu_B}{mc^2} \vec{\sigma} \cdot \vec{B} \hat{H} + \frac{5}{3} \frac{\mu_B Z e^2}{4\pi\epsilon_0 mc^2} \vec{\sigma} \cdot \vec{B} \frac{1}{r} \ . \tag{1.39}$$

Substituting in the fine structure constant α

$$Q_{M1} = \mu_B \vec{\sigma} \cdot \vec{B} + \frac{4}{3} \frac{\mu_B}{mc^2} \vec{\sigma} \cdot \vec{B} \hat{H} + \frac{5}{3} \frac{\mu_B Z \alpha \hbar}{mcr} \vec{\sigma} \cdot \vec{B} \ . \tag{1.40}$$

The Bohr radius a_0 is also substituted into the expression, thus giving the final result

$$Q_{M1} = \mu_B \vec{\sigma} \cdot \vec{B} + \frac{4}{3} \frac{\mu_B}{mc^2} \vec{\sigma} \cdot \vec{B} \hat{H} + \frac{5}{3} \mu_B Z \alpha^2 a_0 \vec{\sigma} \cdot \vec{B} \frac{1}{r} \ . \tag{1.41}$$

The relativistic magnetic dipole moment operator is then written as a perturbation of r^{-1} to the Hamiltonian. Now that the operator has been introduced, the total Zeeman effect for the system can be derived. The total Zeeman effect utilizes not only the electronic Zeeman effect discussed above, but also accounts for the nuclear Zeeman effect. The Hamiltonian for the system now includes the standard definition, the linear electronic Zeeman effect, the quadratic electronic Zeeman effect and the ordinary nuclear Zeeman effect. This is described mathematically as

$$\hat{H}_Z = \frac{e\hbar}{2M} g_I \left[\vec{B} \cdot \vec{\sigma}_N + \frac{M}{m} \left(\frac{g_s}{g_I} Q_{M1} + \frac{B^2 e}{3 g_I \hbar} r^2 \left(P_0(\cos\theta) - P_2(\cos\theta) \right) \right) \right] \tag{1.42}$$

Inserting the Q_{M1} operator into the equation yields

$$\hat{H}_Z = \frac{e\hbar}{2M} g_I \left[\vec{B} \cdot \vec{\sigma}_N + \frac{M}{m} \left(\frac{g_s}{g_I} \mu_B \vec{\sigma} \cdot \vec{B} \left(1 + \frac{4}{3} \frac{\hat{H}}{mc^2} + \frac{5}{3} Z \alpha^2 a_0 \frac{1}{r} \right) + \frac{B^2 e}{3 g_I \hbar} r^2 \right) \right] \tag{1.43}$$

The new Hamiltonian combines previously mentioned effects, and has terms linearly scaling in B, as well as quadratically scaling in B. Several new factors have arisen due to the inclusion of the nuclear magnetic moment such as g_I, the nuclear g-factor, g_s, the electron spin g-factor, and M, the mass of the nucleus. $\vec{\sigma}_N$ is the nuclear spin operator, which is analgous to the electron spin matrices $\vec{\sigma}$. It's subscript is maintained to help distinguish between the nuclear and electronic effects present in the Hamiltonian. Traditionally, the nuclear contribution is ignored as its effect on the system is significantly smaller than the effect present from the electronic terms. The reason the nuclear effect is so much smaller than the electronic effect is because its impact is supressed by the mass of the nucleus. Since the mass of the electron is so much smaller the the nuclear mass, its impact is a factor of $\frac{M}{m}$ stronger than the nuclear effects.

The inclusion of the Q_{M1} operator in the Zeeman effect adds a linear scaling of B to the overall energy of the system. This operator can be combined with the quadratic Zeeman operator discussed previously to yield a relativistic correction to $^3\mathrm{He}^+$. This relativistic correction scales ~~with~~ B^3 and will be the primary focus of this thesis moving forwards. The inclusion of this higher order Zeeman effect adds a small correction to the Zeeman splitting which has since been unnacounted for in high precision magnetometry. The perturbative effects of the relativistic magnetic dipole moment operator is examined below and explores how it modifies the structure of the Hamiltonian.

Within the Q_{M1} operator, it has been shown that the p^2 term can be written in terms of the original Hamiltonian, there is not a need to perform a perturbation about p^2 in order to receive the desired correction to the energy. Thus the perturbation equation for the Q_{M1} operator is

$$\left(H^{(0)} - E^{(0)}\right)|\Psi^{(1)}\rangle = -\left(\frac{5}{3}\mu_B Z\alpha^2 a_0 \frac{1}{r}\vec{\sigma}\cdot\vec{B} - E^{(1)}\right)\frac{e^{-Zr}}{\sqrt{\pi}}\,. \tag{1.44}$$

Similarly to Sec. 1.4, the first order corrected wavefunction is assumed to be of the form of a power series so that the method of Frobenius can be applied[3]. This gives a similar result to the quadratic Zeeman derivation, but the inhomogeneous terms on the right hand side of the equation now correlate to different powers of r.

$$\sum_{j=0}^{\infty}\left[Z(j-1)a_{j-1} - \frac{j(j+1)}{2}a_j\right]r^{j-2} = -\left(\frac{5}{3}\mu_B Z\alpha^2 a_0 \frac{1}{r}\vec{\sigma}\cdot\vec{B} - E^{(1)}\right)\frac{1}{\sqrt{\pi}} \tag{1.45}$$

Where $E^{(1)}$ is defined by equation (??)

$$E^{(1)} = \frac{5}{3}Z^2\alpha^2 a_0 \mu_B \vec{\sigma}\cdot\vec{B} \tag{1.46}$$

[3]Note here that a_0 is the Bohr radius, not the zeroeth term in the sum. Similarly to the derivation for the quadratic Zeeman effect, there is no a_0 term from the summation, and it is determined later. The conflict in notation is avoided for now.

This gives the final result before the recursion relation step

$$\sum_{j=0}^{\infty}\left[Z(j-1)a_{j-1}-\frac{j(j+1)}{2}a_j\right]r^{j-2}=-\frac{5}{3}Z\alpha^2a_0\mu_B\left(\frac{1}{r}-Z\right)\frac{1}{\sqrt{\pi}}\vec{\sigma}\cdot\vec{B} \tag{1.47}$$

The recursion relation is solved once again similarly to that of the quadratic Zeeman perturbation, but this time only a single term in the series appears as nonzero. The first order correction to the hydrogenic wavefunction for a $\frac{1}{r}$ perturbation is

$$|\Psi^{(1)}\rangle = a_0e^{-Zr}+a_1re^{-Zr} \tag{1.48}$$

The a_0 term is determined by the orthogonality imposed on the system once again and the integration yields[4]

$$a_0=-\frac{5}{3}\alpha^2\bar{a_0}\mu_B\vec{\sigma}\cdot\vec{B}\frac{1}{\sqrt{\pi}}\frac{3}{2}\,. \tag{1.49}$$

Thus the final expression for the correction to the hydrogenic wavefunction for a perturbation of the relativistic magnetic dipole operator is

$$|\Psi^{(1)}\rangle = \frac{5}{3}Z\alpha^2a_0\mu_B\vec{\sigma}\cdot\vec{B}\frac{1}{\sqrt{\pi}}e^{-Zr}\left(-\frac{3}{2Z}+r\right) \tag{1.50}$$

Now that the Q_{M1} operator and the quadratic Zeeman operator have been successfully expressed as corrections to the Hamiltonian and its wavefunctions, they can be combined to produce a higher order Zeeman effect scaling with B^3. This combination of Q_{M1} and $H_Z^{(2)}$ is called the relativistic correction, and is discussed in Sec. 1.5.2.

1.5.2 The relativistic correction to $^3He^+$

Combining the relativistic magnetic dipole moment with the quadratic Zeeman operator, the relativistic corrections for $^3He^+$ is uncovered. The relativistic correction

[4]Note that due to the conflicting notation, the Bohr radius is denoted as $\bar{a_0}$.

is

$$C_{\rm rel}^{(2)} = \sum_{n=1}^{\infty} \frac{\langle\psi^0|Q_{M1}|\psi^n\rangle\langle\psi^n|V_Z^{(2)}|\psi^0\rangle}{E_0 - E_n} \ . \tag{1.51}$$

Replacing the infinite sum of the hydrogenic spectrum with the sum over the pseudospectrum for either the quadratic Zeeman operator or the relativistic magnetic dipole operator gives a simplified definition for the relativistic correction. To ensure correctness, both approaches are calculated, and the Dalgarno interchange theorem (see Sec. **??**) is used to verify that both solutions are the same. Starting with the quadratic Zeeman operator, define

$$|\psi^{(1)}\rangle = \sum_{n=1}^{\infty} \frac{|\psi^n\rangle\langle\psi^n|V_Z^{(2)}|\psi^0\rangle}{E_0 - E_n} \ , \tag{1.52}$$

so that the relativistic correction now reads

$$C_{\rm rel}^{(2)} = 2\langle\psi^0|Q_{M1}|\psi^{(1)}\rangle \ . \tag{1.53}$$

$|\psi^{(1)}\rangle$ is also written in equation (1.33), and the solution to $C_{\rm rel}^{(2)}$ is now just an integral

$$C_{\rm rel}^{(2)} = 2\int_0^{\infty}\int_0^{\pi}\int_0^{2\pi} r^2 \sin\theta\psi^0 Q_{M1}\psi^{(1)} dr d\theta d\phi \ . \tag{1.54}$$

expanding ψ^1 and ψ^0 and simplifying

$$C_{\rm rel}^{(2)} = \frac{10}{9}\gamma^2\mu_B\alpha^2 a_0 Z^{\frac{5}{2}} \int_0^{\infty} re^{-2Zr}\left[\frac{11}{2Z^4} - \frac{1}{Z^2}r^2 - \frac{1}{3Z}r^3\right] dr \ \vec{\sigma}\cdot\vec{B} \tag{1.55}$$

Which after integration gives

$$C_{\rm rel}^{(2)} = \frac{5}{6}\gamma^2\mu_B\alpha^2 a_0 Z^{-\frac{7}{2}}\vec{\sigma}\cdot\vec{B} \ . \tag{1.56}$$

It can be seen that the relativistic correction to ^{3}He$^+$ includes a B^3 scaling. This electronic effect further splits the energy levels of ^{3}He$^+$ when subjected to an external magnetic field. The $\vec{\sigma}\cdot\vec{B}$ term ensures that the splitting is dependent on the magnetic quantum number m, so the shift to the energy is a noticeable effect that further increases the splitting between the states. This result is verified using the Dalgarno interchange theorem by defining

$$|\varphi^{(1)}\rangle = \sum_{n=1}^{\infty} \frac{\langle\psi^0|Q_{M1}|\psi^n\rangle\langle\psi^n|}{E_0 - E_n}\ , \tag{1.57}$$

which means that the relativistic correction can also be defined as

$$C_{\rm rel}^{(2)} = 2\langle\varphi|V_Z^{(2)}|\psi^0\rangle\ . \tag{1.58}$$

According to the Dalgarno interchange theorem, this expression for $C_{\rm rel}^{(2)}$ should be the same as the result found in equation (1.56). In integral form this reads

$$C_{\rm rel}^{(2)} = 2\int_0^{\infty}\int_0^{\pi}\int_0^{2\pi} r^2 \sin\theta \frac{5}{3} Z\alpha^2 a_0 \mu_B \vec{\sigma}\cdot\vec{B}\frac{e^{-Zr}}{\sqrt{\pi}}\left[-\frac{3}{2Z} + r\right]\frac{1}{12}\gamma^2 r^2 \frac{Z^{\frac{3}{2}}e^{-Zr}}{\sqrt{\pi}} dr d\theta d\phi\ . \tag{1.59}$$

Which becomes

$$C_{\rm rel}^{(2)} = \frac{5}{6}\gamma^2 \mu_B \alpha^2 a_0 Z^{-\frac{7}{2}} \vec{\sigma}\cdot\vec{B}\ . \tag{1.60}$$

Thus ~~it has been proven via the Dalgarno interchange theorem that all previous calcualtions have been correct, and the relativistic corrections for ^{3}He$^+$ have been successfully derived~~. Reversing the substitution of all of the physical constants one gets

$$C_{\rm rel}^{(2)} = \frac{5}{6}\frac{B^3 e^5 \hbar Z^{\frac{-7}{2}}}{m^3 c^3 4\pi\epsilon_0} m_s\ . \tag{1.61}$$

Which has units of energy per tesla. m_s denotes the magnetic quantum number, which can take values of $\pm\frac{1}{2}$. From this, the further splitting of energy states based on magnetic field strength is evident. The relationship behaves like the splitting shown in figure 1.4.1c. This factor is not supressed by the mass of the nucleus like the ~~other effects~~ discussed in the previous section, and thus ~~becomes impactful to the systems behaviour for all magnitudes of magnetic field~~, regardless of its seemingly small correction.

1.6 RESULTS

This section discusses the numerical results obtained from the calculations of the linear and quadratic Zeeman effects, the relativistic magnetic dipole moment, and the relativistic correction to $^3He^+$ for various magnetic field strengths. The results will highlight the significance of the B^3 term in accounting for the energy level splitting at low and high magnetic field strength.

Magnetic Field Strength	Energy			
Value	$\hat{H}$	$\hat{H}_Z$	$\hat{H}_{\mathrm{Rel}}$	$\hat{H}_{\mathrm{Total}}$
Test	1.0	2.0	3.0	6.0

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[1] Codata value: atomic unit of magnetic flux density.

[2] Codata value: electron mass.

[3] Codata value: elementary charge.

[4] Codata value: fine-structure constant.

[5] Codata value: reduced planck constant.

[6] Codata value: speed of light in vacuum.

[7] Codata value: vacuum electric permittivity.

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