DESCRIBING TWO CHARGED PARTICLES IN A MAGNETIC FIELD USING TRAJECTORIES AND WAVE EQUATIONS THROUGH FACTORIZATION

by

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ABSTRACT

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We examine the nonrelativistic classical equations of motion of two charged massive particles in a static homogeneous magnetic field. We discuss criteria for when the classical nonrelativistic radiationless approximation is valid for this two-particle system. We focus on the motion in the plane perpendicular to the direction of the magnetic field. We determine conditions of boundedness in this plane for both the center-of-mass vector and the relative-position vector that describe the two-particle system. We then examine a spinor equation that describes two nonrelativistic quantum particles in a homogeneous magnetic field. By treating some of the terms of the Hamiltonian as perturbations, we obtain analytic expressions for the energy levels of the two-particle system. We apply these analytic expression to predict the energy levels for neutral two-body systems such as hydrogen and positronium, and for the positive helium ion and any hydrogen-like ions. Finally, we explore a matrix factorization

technique to derive nonrelativistic quantum wave equations which may incorporate spin, and relativistic quantum wave equations which may incorporate anti-particle wave components. From our investigation, we postulate the necessary conditions to obtain Schrödinger wave equations, Pauli wave equations, Klein-Gordon wave equations, and Dirac wave equations.

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Chapter 1

Introduction

1.1 Motivation for this Work

How do two charged particles interact with each other in the presence of an external field? The answer depends on many factors: What is the external field? Are the particles relativistic? Do the particles obey quantum rules? Do the particles have spin? In this thesis, we look at specific cases of two particles interacting with each other in the presence of an external magnetic field, and we provide a mathematical basis of the equations that describe these interactions. First, we investigate two classical particles. The electrostatic force between two classical charged particles is similar to the force of gravity between two bodies.

In the seventeenth century, Newton developed the law of gravity. He stated that the gravitational force between two bodies is inversely proportional to the distance squared. This force describes everything from a ball falling to the Earth to the motion of the planets. A century later, Coulomb discovered that the electrical force between two charged bodies is also inversely proportional to the distance between them squared, and physicists used the electric force to describe the orbit of two

charged particles in much the same way that Newton described the motion of the planets.

These equations of motion based on the electrical force or gravitational force are found in countless textbooks and are well understood. Yet the simple example of analyzing the motion of two classically charged particles in a constant homogenous magnetic field is not generally known.

Chapter 2 examines these motions both analytically and computationally. The addition of a constant homogeneous magnetic field to the motion of two charged particles leads to many surprising and interesting orbits. The analysis begins by describing the system from the center-of-mass and the relative position of the two particles rather than the position of the two particles individually. We define the total pseudomomentum and show that it is a constant vector. We discuss how it is useful to simplify the equations when the two particles have opposite and equal charges. We also define three collective charges: the reduced charge q_r, the total charge q_R, and the interactive charge q_{rR}. These new charge definitions help characterize the resulting motions. Finally, we examine the motion of the particles in the plane parallel to the direction of the external magnetic field, and use the new charge definitions to determine conditions of boundedness.

With the understanding gained in the classical case and the new charges defined in Chapter 2, we are ready to analyze two quantum charged particles with spin in a constant magnetic field in Chapter 3. We use a spinor wave equation that describes both particles jointly rather than using a spinor equation for each particle. We then limit ourselves to two distinguishable particles whose charges have opposite signs. We also assume that the constant magnetic field is weak in order to treat certain terms of the equations as perturbations. With these conditions we obtain the eigenstate energies for the two quantum particles in a constant homogeneous magnetic field. We

recover the results of Reed and Brun [1] for the Zeeman effect of hydrogen and make predictions about the Zeeman effect of a positive helium ion in a magnetic field. The overall analysis illustrates how the appropriate choice of the magnetic vector potential can greatly aid in finding eigenstate energies.

Chapter 3 represents a unique approach to a well-studied problem. In the last sixty years, many papers have been published that investigate the eigenstate energies of atoms in constant homogeneous magnetic and electric fields. We have especially consulted early work by Lamb published in 1952 [2], a thorough treatment by Bruce R. Johnson, Joseph Hirschfelder, and Kuo-Ho Yang published in 1983 [3], and an investigation of ions by P. Schmelcher and L. Cederbaum published in 1991 [4]. All these contributions make use of the concept of total pseudomomentum and treat ions and neutral atoms separately. In contrast, in Chapter 3 we make no reference to the pseudomomentum. We find the eigenvalue energies for both neutral atoms and ions without treating them separately. However, we only look at the particles in a magnetic field, and it is not clear if our approach could be extended to include electric fields, unlike the works cited above.

Chapter 4 uses a matrix factorization technique to derive Schrödinger-like wave equations. The Pauli-like wave equation used to describe the two particles in Chapter 3 was first proposed by Reed and Brun in 2007. Reed and Brun developed a generalized matrix factorization technique to derive quantum wave equations, similar to the technique used by Dirac in 1928 to derive his relativistic wave equation. We use this technique to derive quantum equations for particles with no spin, Pauli-like wave equations for particles with spin, and relativistic equations that do not include antiparticle solutions. This general investigation of the many wave equations available leads us to formulate necessary conditions for obtaining wave equations with spin or wave equations with antiparticle components. Our goal is to gain a better

understanding of the foundations of such equations.

1.2 Notation

Throughout this thesis, we use the following conventions. A caret over any variable, such as $\hat{E}$, indicates that the variable is a quantum operator. All vectors are written in bold but without an arrow; for example, a momentum vector will look like this, $\mathbf{p}$. All equations are written in Gaussian units while the units for numerical values are always explicitly stated.

Chapter 2

Two Classical Particles

2.1 Introduction

We consider the motion of two charged classical particles. First we look at the two charged particles in the absence of an external magnetic field. Then we include a static magnetic field. Finally we look at a homogeneous magnetic field. We study under what conditions the particles are spatially bounded when in the presence of a homogeneous magnetic field and we use numerical simulations to confirm the conditions of boundedness. These results help establish a fundamental basis and understanding which will help us in Chapter 3 to examine two quantum particles in similar situations.

2.2 Assumptions

Throughout this chapter we make four assumptions to simplify our analysis. 1) Relativity can be ignored. 2) The gravitational force between the two particles is small enough that it can be ignored. 3) Energy lost due to radiation can be ignored. 4) Our

system is in the classical regime, and can be modeled without quantum mechanics.

We now examine how these assumptions simplify our analysis and what restrictions they impose on our model.

2.2.1 Relativity Can Be Ignored

To fully understand how nonrelativistic velocities simplify our equations, we look at the relativistic Hamiltonian of two charged particles and see how this Hamiltonian can be reduced by our assumption.

The relativistic Hamiltonian is written in terms of the scalar and vector potentials Φ_1, Φ_2, $\mathbf{A}_1$, and $\mathbf{A}_2$ which describe the electric fields $\mathbf{E}_1$ and $\mathbf{E}_2$ and the magnetic fields $\mathbf{B}_1$ and $\mathbf{B}_2$ that determine the motion of the two particles, where the subscripts 1 and 2 refer to the potentials and fields generated by the first and second particle respectively. The electromagnetic fields are related to the potentials by

$$\mathbf{E}_j = -\nabla\Phi_j - \frac{\partial \mathbf{A}_j}{\partial t}, \quad \mathbf{B}_j = \nabla \times \mathbf{A}_j \tag{2.1}$$

for $j = 1$ or 2. The fields generated by the first particle act at time t_o and radiate out at the speed of light c. These fields arrive at an arbitrary location $\mathbf{r}$ at time t where

$$t - t_o = \frac{|\mathbf{r}(t) - \mathbf{r_1}(t_o)|}{c}. \tag{2.2}$$

Because of this time delay $t - t_o$, it is useful to introduce the following variables

$$R_1 = |\mathbf{r}(t) - \mathbf{r_1}(t_o)|, \tag{2.3}$$

$$\hat{\mathbf{n}} = \frac{\mathbf{r}(t) - \mathbf{r_1}(t_o)}{R_1}. \tag{2.4}$$

With this notation the Lienard-Wiechert potentials created by the first particle of charge q_1 are

$$\Phi_1(\mathbf{r}, t) = \frac{q_1}{\left(1 - \frac{\dot{\mathbf{r}}_1(t_o)}{c} \cdot \hat{\mathbf{n}}\right) R_1}, \quad \mathbf{A}_1(\mathbf{r}, t) = \frac{q_1 \dot{\mathbf{r}}_1(t_o)}{c\left(1 - \frac{\dot{\mathbf{r}}_1(t_o)}{c} \cdot \hat{\mathbf{n}}\right) R_1} \tag{2.5}$$

where $\mathbf{r}_j$ is the position vector of the j^{th} particle and $\dot{\mathbf{r}}_\mathbf{1}(t_o)$ is the time derivative of $\mathbf{r}_j(t)$ evaluated at t_o. Φ_2 and $\mathbf{A}_2$ are defined similarly. With these definitions the Hamiltonian of the two-particle system is [5]

$$H = \sqrt{m_1^2c^4 + (c\mathbf{p}_1 - q_1\mathbf{A}_2)^2} + \sqrt{m_2^2c^4 + (c\mathbf{p}_2 - q_2\mathbf{A}_1)^2} + q_2\Phi_1 + q_1\Phi_2. \tag{2.6}$$

We simplify this Hamiltonian by assuming nonrelativistic velocities. By nonrelativistic velocities, we mean that the velocities of both the particles are much less than the speed of light. In fact, from the perspective of the particles we can assume that the speed of light is infinite. This means that the fields and the vector potentials propagate instantaneously. The potentials generated by the j^{th} particle are then approximated as

$$\Phi_j(\mathbf{r},t) = \frac{q_j}{\left(1 - \frac{\dot{\mathbf{r}}_\mathbf{j}(t_o)}{c}\cdot\hat{\mathbf{n}}\right)R_j} \approx \frac{q_j}{|\mathbf{r}-\mathbf{r}_j|}, \quad \mathbf{A}_j(\mathbf{r},t) = \frac{q_j\dot{\mathbf{r}}_\mathbf{j}(t_o)}{c\left(1 - \frac{\dot{\mathbf{r}}_\mathbf{j}(t_o)}{c}\cdot\hat{\mathbf{n}}\right)R_j} \approx 0. \tag{2.7}$$

Then, using a Taylor approximation of the square root terms found in the Hamiltonian

$$\sqrt{m_j^2c^4 + (c\mathbf{p}_j)^2} \approx m_jc^2\left(1 + \frac{\mathbf{p}_j^2}{m_j^2c^2}\right) \tag{2.8}$$

we obtain

$$H = \frac{{\mathbf{p}_1}^2}{2m_1} + \frac{{\mathbf{p}_2}^2}{2m_2} + \frac{q_1\,q_2}{|\mathbf{r}_1 - \mathbf{r}_2|} + m_1c^2 + m_2c^2, \tag{2.9}$$

or ignoring the rest-mass energies,

$$H = \frac{{\mathbf{p}_1}^2}{2m_1} + \frac{{\mathbf{p}_2}^2}{2m_2} + \frac{q_1\,q_2}{|\mathbf{r}_1 - \mathbf{r}_2|}. \tag{2.10}$$

We have simplified the relativistic Hamiltonian, and we now examine the restrictions we have imposed on our model. We want the two particles to travel much slower than light. By making rough approximations we can obtain a range of values for the mass and charge that should keep the particles in the nonrelativistic regime. We do this by first ignoring the external magnetic field, and by looking at two particles with

charges of opposite sign in bounded motion. After obtaining a range of values for this specific case we extend this same range to all cases. We argue that we can extend our range to two particles with charges of the same sign because such particles repel rather than attract; therefore they are less likely to have close encounters in which the electric force between them would be leading to high velocities. Also, because B-fields do no work, we assume that the addition of the magnetic field will not be able to force our system outside of the nonrelativistic regime in all cases. However if the B-field is strong enough, we might expect that it could cause the two particles to come extremely close, causing the forces between them to increase dramatically, resulting in velocities that approach c.

We can approximate the average speeds of two particles in bounded orbit by dividing the length of the path traveled in one period by the time of one period. The period T of two celestial bodies in a bounded orbit due to gravity is given by Kepler's third law for two physical bodies,

$$T = 2\pi\sqrt{\frac{a^3}{G\left(m_1 + m_2\right)}} \tag{2.11}$$

where a is the sum of the semi-major axis of the orbit of each mass and G is the universal gravitational constant [6]. This can easily be modified to obtain the period of two particles with charges of opposite signs by substituting the gravitational charges m_1 and m_2 with the electrostatic charges q_1 and q_2,

$$T = 2\pi\sqrt{\frac{a^3\mu}{-q_1 q_2}} \tag{2.12}$$

where μ is the reduced mass

$$\mu = \frac{m_1 m_2}{m_1 + m_2}. \tag{2.13}$$

We take the magnitude of the distance traveled by the j^{th} particle to be $2\pi a$. This overestimates the true distance traveled by the j^{th} particle because a is the sum of

the semi-major axis of orbit, but for our purposes it will do. We get as the average velocity for each particle

$$v_{avg} = \sqrt{\frac{-q_1 q_2}{\mu a}}. \tag{2.14}$$

In order to stay in the nonrelativistic regime we require that the average speed be much less than the speed of light, so that at any given time the velocity of the j^{th} particle is much less than c

$$\frac{|q_1 q_2|}{\mu} \ll ac^2. \tag{2.15}$$

If we consider the hydrogen atom and use the Bohr radius for a, we obtain

$$\frac{|q_1 q_2|}{\mu} = 253\,\frac{m^3}{s^2} \qquad ac^2 = 4.77 * 10^6\,\frac{m^3}{s^2}. \tag{2.16}$$

The hydrogen atom clearly satisfies Eq.(2.15).

2.2.2 Gravity Can Be Ignored

In our simulations we do not want the gravitational force between the two particles to be nearly as strong as the electric force because we neglect gravity in all our equations. Therefore, we require

$$\frac{Gm_1 m_2}{r^2} \ll \frac{|q_1 q_2|}{r^2}. \tag{2.17}$$

Combining this criterion with Eq.(2.15) we have

$$GM \ll \frac{|q_1 q_2|}{\mu} \ll ac^2 \tag{2.18}$$

where M is the total mass $M = m_1 + m_2$. If we consider the hydrogen atom, we obtain

$$Gm_1 m_2 = 1.02 * 10^{-67}\,kg\frac{m^3}{s^2} \qquad |q_1 q_2| = 2.30 * 10^{-28}\,kg\frac{m^3}{s^2}. \tag{2.19}$$

If both the electron and proton were each 10^{20} times more massive than they actually are, the gravitational force between them would be about five times greater than the electrical force between them.

2.2.3 Radiation Can Be Ignored

Accelerating charges radiate; however our model will not take that into account. The power radiated for a nonrelativistic particle is given by Larmor's formula [5]

$$P = \frac{2q^2\ddot{r}^2}{3c^3} \tag{2.20}$$

where $\ddot{r}$ is the particle's acceleration. For our model to be accurate we want the total energy radiated in one orbit to be a small fraction of the kinetic energy of the particle. We take T to be the period of one orbit; v_{avg}^2 is the average velocity squared of the particle and $\ddot{r}_{avg}^2$ is the average acceleration squared of the particle. For both particles we want

$$PT = \frac{2q^2\ddot{r}_{avg}^2}{3c^3}T \ll \frac{1}{2}mv_{avg}^2. \tag{2.21}$$

We consider the electron of a hydrogen atom and assume that the electron moves in a circular orbit with a radius equal to Bohr's radius. For circular orbits we know that $\ddot{r}^2 = \frac{\dot{r}^2}{a}$, where a is the radius. From the electric force law we also know that $\ddot{r}^2 = \left|\frac{q_1 q_2}{a^2 m_1}\right|$, where m_1 is the mass of an electron and q_1 and q_2 are the charges of the electron and proton respectively. We can write T, the period of one orbit, as $T = \frac{2\pi a}{\dot{r}}$. We obtain

$$\frac{2q^2\ddot{r}_{avg}^2}{3c^3}T = \frac{4\pi q^5}{3c^3 a^{5/2} m_1^{3/2}} = 7.07 * 10^{-24} J \tag{2.22}$$

$$\frac{1}{2}mv_{avg}^2 = \frac{q^2}{a} = 2.177 * 10^{-18} J. \tag{2.23}$$

This satisfies Eq.(2.21), which means that if hydrogen obeyed classical trajectories, we could model the hydrogen atom accurately for many orbits without considering radiation. However there is a problem with modeling hydrogen in this manner. Even though in each orbit the electron radiates approximately only 10^{-5} of its kinetic energy, the period of one orbit is $T = 1.52 * 10^{-16}$ seconds, and in less than a second it will radiate all of its kinetic energy. Using this model of hydrogen would lead us

to believe that the life-time of the hydrogen atom is less than a second, which is not true. The electron in the hydrogen atom stops radiating once it reaches the ground state, which is predicted by quantum mechanics.

2.2.4 Quantum Mechanics Can Be Ignored

In order to ignore quantum mechanics we would like to deal with a system where the eigenstate energies are essentially continuous. In other words, we want the energy of the system to be high enough so that the difference between consecutive eigenstate energies around the energy is essentially zero. Unfortunately, we cannot know what the eigenstate energies are until we actually solve the quantum wave equations that describe the system. However, if we work under the assumption that the difference between consecutive eigenstate energies is similar to the difference found in a hydrogen-like atom, we can create a rough criterion to ensure that quantum mechanics can be ignored. We use the hydrogen-like atom because the eigenstate energies are already known. Also, if we ignore the magnetic field and assume that our particles have charges of opposite sign, our system becomes a hydrogen-like atom. The eigenstate energies of the hydrogen-like atom are

$$E_n = -\frac{\mu \left|q_1 q_2\right|^2}{2\hbar^2 n^2} \tag{2.24}$$

where n is an integer, and $\hbar$ is Planck's constant divided by 2π. As $n \to \infty$ the difference between consecutive eigenstate energies goes to zero. For a classical system the total energy is $E = V + E_k$, where V is the potential energy and E_k is the total kinetic energy. We can find what n must be to obtain this energy:

$$n = \sqrt{\frac{\mu \left|q_1 q_2\right|^2}{2\hbar^2 \left|E\right|}}. \tag{2.25}$$

The higher n is, the less need there is to consider quantum mechanics. For this work, we will consider it safe to assume that quantum mechanics can be ignored if $n > 10^6$.

In other words, our criterion is

$$\sqrt{\frac{\mu \left|q_1 q_2\right|^2}{2\hbar^2 \left|E\right|}} > 10^6. \tag{2.26}$$

The criterion of $n > 10^6$ in this thesis is much stricter than that found in other work. Hydrogen atoms where $n \approx 100$ are considered Rydberg atoms and are often approximated using classical trajectories [7].

2.3 Motion with No Magnetic Field

The classical problem of obtaining equations of motion for two charged particles with no magnetic field has a well-known solution based on a coordinate transformation. We begin by transforming from the $\mathbf{r}_1$ and $\mathbf{r}_2$ position vectors to the relative-position vector $\mathbf{r}$ and center-of-mass position vector $\mathbf{R}$ by the relations

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2 \quad \text{and} \quad \mathbf{R} = \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1 + m_2}. \tag{2.27}$$

Under these transformations, we obtain a new expression for the Hamiltonian in Eq.(2.10)

$$H = \frac{\mathbf{p}^2}{2\mu} + \frac{\mathbf{P}^2}{2M} + \frac{q_1\, q_2}{|\mathbf{r}|}, \tag{2.28}$$

where the Hamiltonian is written in terms of the reduced mass μ and the total mass M and the new momenta $\mathbf{p}$ and $\mathbf{P}$.

$$\mu = \frac{m_1 m_2}{m_1 + m_2} \quad , \quad M = m_1 + m_2 \ , \tag{2.29}$$

$$\mathbf{p} = \frac{m_2\mathbf{p}_1 - m_1\mathbf{p}_2}{m_1 + m_2} \quad \text{and} \quad \mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2. \tag{2.30}$$

We notice that since the potential energy only depends on one of the position vectors we can separate the Hamiltonian into two parts

$$H_{\mathbf{r}} = \frac{\mathbf{p}^2}{2\mu} + \frac{q_1\, q_2}{|\mathbf{r}|} \quad \text{and} \quad H_{\mathbf{R}} = \frac{\mathbf{P}^2}{2M}. \tag{2.31}$$

This leads to separate independent equations of motions for $\mathbf{r}$ and $\mathbf{R}$ [8].

2.4 Motion in a Static Magnetic Field

The Hamiltonian for two charged nonrelativistic particles of charge q_1 and q_2 in a static external magnetic field $\mathbf{B}$ can be obtained by a small modification of Eq.(2.10)

$$H = \frac{\left(\mathbf{p}_1 - \frac{q_1}{c}\mathbf{A}\left(\mathbf{r}_1\right)\right)^2}{2m_1} + \frac{\left(\mathbf{p}_2 - \frac{q_2}{c}\mathbf{A}\left(\mathbf{r}_2\right)\right)^2}{2m_2} + \frac{q_1\, q_2}{|\mathbf{r}_1 - \mathbf{r}_2|} \tag{2.32}$$

where $\mathbf{A}\left(\mathbf{r}_j\right)$ is the vector potential associated with the external magnetic field and satisfies

$$\mathbf{B} = \nabla \times \mathbf{A}. \tag{2.33}$$

We could obtain the equations of motion for $\mathbf{r}_1$ and $\mathbf{r}_2$ using Hamiltonian's equation. However, in this particular case it is simpler to use the Lorentz force law, which reveals

$$m_1\, \ddot{\mathbf{r}}_1 = \frac{q_1}{c}\, \dot{\mathbf{r}}_{\mathbf{1}} \times \mathbf{B} + \frac{q_1\, q_2}{|\mathbf{r}_1 - \mathbf{r}_2|^{\frac{3}{2}}}\left(\mathbf{r}_1 - \mathbf{r}_2\right), \tag{2.34}$$

$$m_2\, \ddot{\mathbf{r}}_2 = \frac{q_2}{c}\, \dot{\mathbf{r}}_{\mathbf{2}} \times \mathbf{B} + \frac{q_1\, q_2}{|\mathbf{r}_1 - \mathbf{r}_2|^{\frac{3}{2}}}\left(\mathbf{r}_2 - \mathbf{r}_1\right). \tag{2.35}$$

Solving these two coupled equations for $\mathbf{r}_1$ and $\mathbf{r}_2$ is difficult because the $|\mathbf{r}_1 - \mathbf{r}_2|^{\frac{3}{2}}$ term in the denominator of the electric force term in both equations makes eliminating $\mathbf{r}_1$ or $\mathbf{r}_2$ in either equation impossible. In the two-particle system without an external field, the solution to a similar problem was found in transforming coordinates from $\mathbf{r}_1$ and $\mathbf{r}_2$ to $\mathbf{r}$ and $\mathbf{R}$. Let us try this approach. Following the transformations given by Eq.(2.29) and Eq.(2.30) we find the Hamiltonian from Eq.(2.32)

$$H = \frac{\left(\mathbf{p} - \left[\frac{m_2}{M}\frac{q_1}{c}\mathbf{A}\left(\mathbf{r}_1\right) - \frac{m_1}{M}\frac{q_2}{c}\mathbf{A}\left(\mathbf{r}_2\right)\right]\right)^2}{2\mu} + \frac{\left(\mathbf{P} - \left[\frac{q_1}{c}\mathbf{A}\left(\mathbf{r}_1\right) + \frac{q_2}{c}\mathbf{A}\left(\mathbf{r}_2\right)\right]\right)^2}{2M} + \frac{q_1\, q_2}{|\mathbf{r}|}. \tag{2.36}$$

Upon eliminating $\mathbf{r}_1$ and $\mathbf{r}_2$ with Eq.(2.27) we have

$$H = \frac{\left(\mathbf{p}-\left[\frac{m_2}{M}\frac{q}{c}\mathbf{A}\left(\mathbf{R}+\frac{m_2}{M}\mathbf{r}\right)-\frac{m_1}{M}\frac{q_2}{c}\mathbf{A}\left(\mathbf{R}-\frac{m_1}{M}\mathbf{r}\right)\right]\right)^2}{2\mu} + \frac{\left(\mathbf{P}-\left[\frac{q_1}{c}\mathbf{A}\left(\mathbf{R}+\frac{m_2}{M}\mathbf{r}\right)+\frac{q_2}{c}\mathbf{A}\left(\mathbf{R}-\frac{m_1}{M}\mathbf{r}\right)\right]\right)^2}{2M} + \frac{q_1 q_2}{|\mathbf{r}|}. \tag{2.37}$$

We can now solve for the equations of motion using Hamilton's equations

$$-\dot{p}_j = \frac{\partial H}{\partial r_j} \text{ and } \dot{r}_j = \frac{\partial H}{\partial p_j}. \tag{2.38}$$

Before we do this it is useful to introduce some new variables. First we redefine the vector potentials

$$\mathbf{A}_{\mathbf{r}}(\mathbf{r},\mathbf{R}) = \frac{m_2}{M}\frac{q_1}{c}\mathbf{A}\left(\mathbf{R}+\frac{m_2}{M}\mathbf{r}\right) - \frac{m_1}{M}\frac{q_2}{c}\mathbf{A}\left(\mathbf{R}-\frac{m_1}{M}\mathbf{r}\right), \tag{2.39}$$

$$\mathbf{A}_{\mathbf{R}}(\mathbf{r},\mathbf{R}) = \frac{q_1}{c}\mathbf{A}\left(\mathbf{R}+\frac{m_2}{M}\mathbf{r}\right) + \frac{q_2}{c}\mathbf{A}\left(\mathbf{R}-\frac{m_1}{M}\mathbf{r}\right) \tag{2.40}$$

where we have included $\frac{q_j}{c}$ in the definition of the new vector potentials. We will not only use these new vector potentials in the equations of motion but also their derivatives with respect to $\mathbf{r}$ and $\mathbf{R}$.

$$\frac{\partial}{\partial r_j}\mathbf{A}_{\mathbf{r}}(\mathbf{r},\mathbf{R}) = \frac{m_2}{M}\frac{q_1}{c}\frac{\partial}{\partial r_j}\mathbf{A}\left(\mathbf{R}+\frac{m_2}{M}\mathbf{r}\right) - \frac{m_1}{M}\frac{q_2}{c}\frac{\partial}{\partial r_j}\mathbf{A}\left(\mathbf{R}-\frac{m_1}{M}\mathbf{r}\right) \tag{2.41}$$

which simplifies to

$$\frac{\partial}{\partial r_j}\mathbf{A}_{\mathbf{r}}(\mathbf{r},\mathbf{R}) = \left(\frac{m_2}{M}\right)^2\frac{q_1}{c}\mathbf{A}^{j'}\left(\mathbf{R}+\frac{m_2}{M}\mathbf{r}\right) + \left(\frac{m_1}{M}\right)^2\frac{q_2}{c}\mathbf{A}^{j'}\left(\mathbf{R}-\frac{m_1}{M}\mathbf{r}\right) \tag{2.42}$$

where

$$\mathbf{A}^{j'}(\mathbf{h}) = \frac{\partial \mathbf{A}(\mathbf{h})}{\partial h_j}. \tag{2.43}$$

The superscript j' in Eq.(2.43) represents the vector component with respect to which the partial derivative is taken. In a similar way, we find the other derivatives

$$\frac{\partial}{\partial R_j}\mathbf{A}_{\mathbf{R}}(\mathbf{r},\mathbf{R}) = \frac{q_1}{c}\mathbf{A}^{j'}\left(\mathbf{R}+\frac{m_2}{M}\mathbf{r}\right) + \frac{q_2}{c}\mathbf{A}^{j'}\left(\mathbf{R}-\frac{m_1}{M}\mathbf{r}\right), \tag{2.44}$$

$$\frac{\partial}{\partial r_j}\mathbf{A}_{\mathbf{R}}\left(\mathbf{r},\mathbf{R}\right)=\frac{m_2}{M}\frac{q_1}{c}\,\mathbf{A}^{j'}\left(\mathbf{R}+\frac{m_2}{M}\mathbf{r}\right)-\frac{m_1}{M}\frac{q_2}{c}\,\mathbf{A}^{j'}\left(\mathbf{R}-\frac{m_1}{M}\mathbf{r}\right), \tag{2.45}$$

$$\frac{\partial}{\partial R_j}\mathbf{A}_{\mathbf{r}}\left(\mathbf{r},\mathbf{R}\right)=\frac{m_2}{M}\frac{q_1}{c}\,\mathbf{A}^{j'}\left(\mathbf{R}+\frac{m_2}{M}\mathbf{r}\right)-\frac{m_1}{M}\frac{q_2}{c}\,\mathbf{A}^{j'}\left(\mathbf{R}-\frac{m_1}{M}\mathbf{r}\right). \tag{2.46}$$

This motivates the definition of the following new expressions

$$\mathbf{A}_{\mathbf{r}}^{j'}=\frac{\partial}{\partial r_j}\mathbf{A}_{\mathbf{r}}\left(\mathbf{r},\mathbf{R}\right), \tag{2.47}$$

$$\mathbf{A}_{\mathbf{R}}^{j'}=\frac{\partial}{\partial R_j}\mathbf{A}_{\mathbf{R}}\left(\mathbf{r},\mathbf{R}\right), \tag{2.48}$$

$$\mathbf{A}_{\mathbf{rR}}^{j'}=\frac{\partial}{\partial r_j}\mathbf{A}_{\mathbf{R}}\left(\mathbf{r},\mathbf{R}\right)=\frac{\partial}{\partial R_j}\mathbf{A}_{\mathbf{r}}\left(\mathbf{r},\mathbf{R}\right). \tag{2.49}$$

With this new notation we obtain the following equations of motion

$$\dot{\mathbf{r}}=\frac{1}{\mu}\left(\mathbf{p}-\mathbf{A}_{\mathbf{r}}\left(\mathbf{r},\mathbf{R}\right)\right), \tag{2.50}$$

$$\dot{\mathbf{R}}=\frac{1}{M}\left(\mathbf{P}-\mathbf{A}_{\mathbf{R}}\left(\mathbf{r},\mathbf{R}\right)\right), \tag{2.51}$$

$$\dot{p}_j=\dot{\mathbf{r}}\cdot\mathbf{A}_{\mathbf{r}}^{j'}+\dot{\mathbf{R}}\cdot\mathbf{A}_{\mathbf{rR}}^{j'}+\frac{q_1\,q_2\,r_j}{\left|\mathbf{r}\right|^3}, \tag{2.52}$$

$$\dot{P}_j=\dot{\mathbf{r}}\cdot\mathbf{A}_{\mathbf{rR}}^{j'}+\dot{\mathbf{R}}\cdot\mathbf{A}_{\mathbf{R}}^{j'}. \tag{2.53}$$

We can rewrite Eq.(2.52) and Eq.(2.53) in matrix form

$$\dot{\mathbf{p}}=\mathcal{A}_{\mathbf{r}}^{'}\,\dot{\mathbf{r}}+\mathcal{A}_{\mathbf{rR}}^{'}\,\dot{\mathbf{R}}+\frac{q_1\,q_2}{\left|\mathbf{r}\right|^2}\hat{\mathbf{r}}, \tag{2.54}$$

$$\dot{\mathbf{P}}=\mathcal{A}_{\mathbf{rR}}^{'}\,\dot{\mathbf{r}}+\mathcal{A}_{\mathbf{R}}^{'}\,\dot{\mathbf{R}}, \tag{2.55}$$

where in a Cartesian coordinate system

$$\dot{\mathbf{p}}=\begin{pmatrix}\dot{p}_x\\ \dot{p}_y\\ \dot{p}_z\end{pmatrix} \tag{2.56}$$

and $\dot{\mathbf{r}}$, $\hat{\mathbf{r}}$, $\dot{\mathbf{P}}$, and $\dot{\mathbf{R}}$ are defined similarly, $\hat{\mathbf{r}}$ being the unit vector of $\mathbf{r}$, and where the matrices $\mathcal{A}'_{\mathbf{r}}$, $\mathcal{A}'_{\mathbf{R}}$, and $\mathcal{A}'_{\mathbf{rR}}$ have the following form

$$\mathcal{A}'_{\mathbf{j}} = \begin{pmatrix} A^{x'}_{\mathbf{j}\,x} & A^{x'}_{\mathbf{j}\,y} & A^{x'}_{\mathbf{j}\,z} \\ A^{y'}_{\mathbf{j}\,x} & A^{y'}_{\mathbf{j}\,y} & A^{y'}_{\mathbf{j}\,z} \\ A^{z'}_{\mathbf{j}\,x} & A^{z'}_{\mathbf{j}\,y} & A^{z'}_{\mathbf{j}\,z} \end{pmatrix}. \tag{2.57}$$

Here the first subscript $\mathbf{j}$ represents the vector potential with which we are dealing and can be either $\mathbf{R}$, $\mathbf{r}$, or $\mathbf{rR}$. The second subscript represents the Cartesian component of the vector potential. We can eliminate $\dot{\mathbf{p}}$ and $\dot{\mathbf{P}}$ by taking the time derivative of Eq. (2.50) and Eq. (2.51) where

$$\frac{d}{dt}\mathbf{A}_{\mathbf{r}}(\mathbf{r},\mathbf{R}) = \begin{pmatrix} A^{x'}_{\mathbf{r}\,x} & A^{y'}_{\mathbf{r}\,x} & A^{z'}_{\mathbf{r}\,x} \\ A^{x'}_{\mathbf{r}\,y} & A^{y'}_{\mathbf{r}\,y} & A^{z'}_{\mathbf{r}\,y} \\ A^{x'}_{\mathbf{r}\,z} & A^{y'}_{\mathbf{r}\,z} & A^{z'}_{\mathbf{r}\,z} \end{pmatrix} \begin{pmatrix} \dot{r}_x \\ \dot{r}_y \\ \dot{r}_z \end{pmatrix} + \begin{pmatrix} A^{x'}_{\mathbf{rR}\,x} & A^{y'}_{\mathbf{rR}\,x} & A^{z'}_{\mathbf{rR}\,x} \\ A^{x'}_{\mathbf{rR}\,y} & A^{y'}_{\mathbf{rR}\,y} & A^{z'}_{\mathbf{rR}\,y} \\ A^{x'}_{\mathbf{rR}\,z} & A^{y'}_{\mathbf{rR}\,z} & A^{z'}_{\mathbf{rR}\,z} \end{pmatrix} \begin{pmatrix} \dot{R}_x \\ \dot{R}_y \\ \dot{R}_z \end{pmatrix} \tag{2.58}$$

which can be written concisely as

$$\frac{d}{dt}\mathbf{A}_{\mathbf{r}}(\mathbf{r},\mathbf{R}) = \mathcal{A}'^{\dagger}_{\mathbf{r}}\dot{\mathbf{r}} + \mathcal{A}'^{\dagger}_{\mathbf{rR}}\dot{\mathbf{R}} \tag{2.59}$$

where $\dagger$ indicates the transpose of a matrix. The time derivative of Eq.(2.50) is

$$\mu\,\ddot{\mathbf{r}} + \mathcal{A}'^{\dagger}_{\mathbf{r}}\dot{\mathbf{r}} + \mathcal{A}'^{\dagger}_{\mathbf{rR}}\dot{\mathbf{R}} = \dot{\mathbf{p}}. \tag{2.60}$$

Upon substitution in Eq.(2.54) we obtain

$$\mu\,\ddot{\mathbf{r}} = \left(\mathcal{A}'_{\mathbf{r}} - \mathcal{A}'^{\dagger}_{\mathbf{r}}\right)\dot{\mathbf{r}} + \left(\mathcal{A}'_{\mathbf{rR}} - \mathcal{A}'^{\dagger}_{\mathbf{rR}}\right)\dot{\mathbf{R}} + \frac{q_1\,q_2}{|\mathbf{r}|^2}\hat{\mathbf{r}}. \tag{2.61}$$

And similarly,

$$M\,\ddot{\mathbf{R}} = \left(\mathcal{A}'_{\mathbf{R}} - \mathcal{A}'^{\dagger}_{\mathbf{R}}\right)\dot{\mathbf{R}} + \left(\mathcal{A}'_{\mathbf{rR}} - \mathcal{A}'^{\dagger}_{\mathbf{rR}}\right)\dot{\mathbf{r}}. \tag{2.62}$$

In general, Eq.(2.61) and Eq.(2.62) cannot be solved analytically. In the case of a static homogeneous magnetic field Eq.(2.61) and Eq.(2.62) can be simplified.

2.5 Motion in a Homogeneous Magnetic Field

Let us consider a static homogeneous magnetic field. We will orient the z-axis along the field of strength B,

$$\mathbf{B} = (0, 0, B)\,. \tag{2.63}$$

For the vector potential we choose the symmetric gauge

$$\mathbf{A} = \frac{1}{2} B\ (-x, y, 0)\,. \tag{2.64}$$

All the $\mathcal{A}'_{\mathbf{j}}$ matrices in Eq.(2.61) and Eq.(2.62) can be written as a constant times a single matrix $\mathcal{A}'$ with physical dimensions of a magnetic field,

$$\mathcal{A}' = \frac{B}{2} \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{2.65}$$

$$\mathcal{A}'_{\mathbf{r}} = \left[\left(\frac{m_2}{M} \right)^2 \frac{q_1}{c} + \left(\frac{m_1}{M} \right)^2 \frac{q_2}{c} \right] \mathcal{A}' \tag{2.66}$$

$$\mathcal{A}'_{\mathbf{R}} = \frac{q_1 + q_2}{c}\, \mathcal{A}' \tag{2.67}$$

$$\mathcal{A}'_{\mathbf{rR}} = \frac{m_2\, q_1 - m_1\, q_2}{M\, c}\, \mathcal{A}'. \tag{2.68}$$

These coefficients have dimensions of charge divided by c. This makes sense because in Eq.(2.40) we absorbed these constants into our definition of new vector potentials $\mathbf{A_r}\,(\mathbf{r}, \mathbf{R})$ and $\mathbf{A_R}\,(\mathbf{r}, \mathbf{R})$. We define the following mathematical charges

$$q_r = \frac{m_2^2\, q_1 + m_1^2\, q_2}{M^2}\ ,\ q_R = q_1 + q_2\ ,\ q_{rR} = \frac{m_2\, q_1 - m_1\, q_2}{M} \tag{2.69}$$

which we name: the reduced charge, the total charge, and the interactive charge respectively. The reduced charged is so named because it is associated with the reduced mass. The total charge is associated with the total mass. And the interactive

charge is the charge that couples the center-of-mass vector to the relative-position vector.

The equations of motion for the center-of-mass vector and relative-position vector are

$$\mu\,\ddot{\mathbf{r}} = \frac{B}{c}\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\left(q_r\,\dot{\mathbf{r}} + q_{rR}\,\dot{\mathbf{R}}\right) + \frac{q_1\,q_2}{|\mathbf{r}|^2}\hat{\mathbf{r}}, \tag{2.70}$$

$$M\,\ddot{\mathbf{R}} = \frac{B}{c}\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\left(q_R\dot{\mathbf{R}} + q_{rR}\dot{\mathbf{r}}\right). \tag{2.71}$$

This can be written

$$\mu\,\ddot{\mathbf{r}} = \frac{q_r}{c}\,\dot{\mathbf{r}}\times\mathbf{B} + \frac{q_{rR}}{c}\,\dot{\mathbf{R}}\times\mathbf{B} + \frac{q_1\,q_2}{|\mathbf{r}|^2}\hat{\mathbf{r}}, \tag{2.72}$$

$$M\,\ddot{\mathbf{R}} = \frac{q_R}{c}\,\dot{\mathbf{R}}\times\mathbf{B} + \frac{q_{rR}}{c}\,\dot{\mathbf{r}}\times\mathbf{B}. \tag{2.73}$$

Eq.(2.72) and Eq.(2.73) are written in terms of q_r, q_R and q_{rR} instead of q_1 and q_2 except for the electric force term $\frac{q_1\,q_2}{|\mathbf{r}|^2}\hat{\mathbf{r}}$ in Eq.(2.72). We can express $q_1\,q_2$ in terms of q_R and q_{rR}. We have

$$q_1 = q_R - q_2 \tag{2.74}$$

and

$$q_2 = \frac{-Mq_{rR} + m_2q_1}{m_1}. \tag{2.75}$$

Combining these equations yields

$$q_1 = \frac{m_1}{M}q_R + q_{rR}. \tag{2.76}$$

In a similar matter we obtain

$$q_2 = \frac{m_2}{M}q_R - q_{rR}. \tag{2.77}$$

Therefore,

$$q_1 q_2 = \frac{\mu}{M} q_R^2 + q_R q_{rR} \left(\frac{m_2 - m_1}{M} \right) - q_{rR}^2. \tag{2.78}$$

We can also express $q_1 q_2$ in terms of q_r and q_{rR},

$$q_1 = \frac{M}{m_2} q_r + \frac{m_1}{m_2} q_{rR}. \tag{2.79}$$

$$q_2 = \frac{M}{m_1} q_r - \frac{m_2}{m_1} q_{rR}. \tag{2.80}$$

$$q_1 q_2 = \frac{M}{\mu} q_r^2 + q_r q_{rR} \left(\frac{m_1 - m_2}{\mu} \right) - q_{rR}^2. \tag{2.81}$$

However, we cannot express $q_1 q_2$ in terms of q_R and q_r. For example, consider the case where $m_1 = m_2$ and $q_1 = -q_2$, this gives $q_R = q_r = 0$. Any combination of q_R and q_r will not give $q_1 q_2 = -q_1^2$. Throughout the rest of this thesis we will not replace $q_1 q_2$ with the expressions found in Eq.(2.78) or Eq.(2.81) because $q_1 q_2$ is simpler.

In this derivation we defined many new variables, but the results found in Eq.(2.72) and Eq.(2.73) are quite simple to interpret. They quickly yield many results that otherwise would be hard to predict. For example, if $m_2\, q_1 = m_1\, q_2$, then $q_{rR} = 0$ and the motion of the center-of-mass vector is no longer coupled to the motion of the relative-position vector. The center-of-mass vector will then move exactly as a particle of mass M and charge q_R would do in the same magnetic field.

We can imagine that the center-of-mass and relative-position vectors are describing the position of real particles except for the q_{rR} term. The center-of-mass and relative-position vectors act as though they were two fictitious particles of masses M and μ and charges q_R and q_r in the same magnetic field as the real particles one and two. The relative-position vector also moves as if it were in a potential well created by the two charges q_1 and q_2, whereas the center of mass is in no such potential. Finally, both mathematical particles are coupled together by the cross product of the velocities of one another with the B-field. This coupling is proportional to the interactive

charge q_{rR}. This last interaction appears to be purely the result of the coordinate transformation with no real physical system counterpart.

However, we can physically explain why the coupled charge q_{rR} found in Eq.(2.72) is the same as that found in Eq.(2.73). To do this, we first note that the system we are dealing with is conservative. The two-particle system without an external magnetic field is an isolated system which has a constant total energy, and the addition of a magnetic field does not change that because a magnetic field can do no work. In a conservative system the net change in energy over any given time period is zero. In the $\mathbf{r}$ and $\mathbf{R}$ view of the system, this can be written as

$$\frac{1}{2}\mu \triangle \dot{\mathbf{r}}^2 + \frac{1}{2}M \triangle \dot{\mathbf{R}}^2 + \triangle V(\mathbf{r}) = 0 \tag{2.82}$$

where $V(\mathbf{r})$ is the electric potential and $\triangle$ indicates the change of these quantities over some finite time. If Eq.(2.72) and Eq.(2.73) contained different coupled charges q_{rR} and q_{Rr} then

$$\mu\, \ddot{\mathbf{r}} = \frac{q_r}{c}\, \dot{\mathbf{r}} \times \mathbf{B} + \frac{q_{rR}}{c}\, \dot{\mathbf{R}} \times \mathbf{B} + \frac{q_1\, q_2}{|\mathbf{r}|^2}\hat{\mathbf{r}} \tag{2.83}$$

$$M\, \ddot{\mathbf{R}} = \frac{q_R}{c}\, \dot{\mathbf{R}} \times \mathbf{B} + \frac{q_{Rr}}{c}\, \dot{\mathbf{r}} \times \mathbf{B}. \tag{2.84}$$

By taking the dot product of Eq.(2.83) with $\dot{\mathbf{r}}$ and the dot product of Eq.(2.84) with $\dot{\mathbf{R}}$ and use the vector identity $\mathbf{A} \cdot (\mathbf{A} \times \mathbf{B}) = 0$, we obtain

$$\mu\, \ddot{\mathbf{r}} \cdot \dot{\mathbf{r}} = \frac{q_{rR}}{c}\, \dot{\mathbf{r}} \cdot \left(\dot{\mathbf{R}} \times \mathbf{B}\right) + \frac{q_1\, q_2}{|\mathbf{r}|^2}\hat{\mathbf{r}} \cdot \dot{\mathbf{r}}, \tag{2.85}$$

$$M\, \ddot{\mathbf{R}} \cdot \dot{\mathbf{R}} = \frac{q_{Rr}}{c}\, \dot{\mathbf{R}} \cdot (\dot{\mathbf{r}} \times \mathbf{B}). \tag{2.86}$$

Now we add Eq.(2.85) to Eq.(2.86), rearrange the terms, and use the vector property $\mathbf{A} \cdot (\mathbf{B} \times \mathbf{C}) = -\mathbf{B} \cdot (\mathbf{A} \times \mathbf{C})$ to obtain

$$\mu\, \ddot{\mathbf{r}} \cdot \dot{\mathbf{r}} + M\, \ddot{\mathbf{R}} \cdot \dot{\mathbf{R}} - \frac{q_1\, q_2}{|\mathbf{r}|^2}\hat{\mathbf{r}} \cdot \dot{\mathbf{r}} = \left(\frac{q_{rR}}{c} - \frac{q_{Rr}}{c}\right) \dot{\mathbf{r}} \cdot \left(\dot{\mathbf{R}} \times \mathbf{B}\right). \tag{2.87}$$

Integrating both sides of the equation over time gives

$$\frac{1}{2}\mu \triangle \dot{\mathbf{r}}^2 + \frac{1}{2}M \triangle \dot{\mathbf{R}}^2 + \triangle V(\mathbf{r}) = \left(\frac{q_{rR}}{c} - \frac{q_{Rr}}{c}\right) \int_0^t \dot{\mathbf{r}} \cdot \left(\dot{\mathbf{R}} \times \mathbf{B}\right) \, dt. \tag{2.88}$$

Now comparing equation Eq.(2.82) and Eq.(2.88) reveals immediately that

$$\left(\frac{q_{rR}}{c} - \frac{q_{Rr}}{c}\right) \int_0^t \dot{\mathbf{r}} \cdot \left(\dot{\mathbf{R}} \times \mathbf{B}\right) \, dt = 0 \tag{2.89}$$

which means that either $q_{rR} = q_{Rr}$ or $\int_0^t \dot{\mathbf{r}} \cdot \left(\dot{\mathbf{R}} \times \mathbf{B}\right) \, dt = 0$ or both. If we are to assume the integral is zero for any time t then we simply look at a time t where $\dot{\mathbf{r}} \cdot \left(\dot{\mathbf{R}} \times \mathbf{B}\right)$ never changes signs and we conclude that $\dot{\mathbf{r}} \cdot \left(\dot{\mathbf{R}} \times \mathbf{B}\right) = 0$. However we can simply choose initial conditions such that $\dot{\mathbf{r}} \cdot \left(\dot{\mathbf{R}} \times \mathbf{B}\right) \neq 0$ at $t = 0$. Therefore $q_{rR} = q_{Rr}$.

2.6 Pseudomomentum

Because the magnetic field $\mathbf{B}$ is constant in time, Eq.(2.73) can be integrated in time and rewritten in terms of the total time derivative of a constant vector $\mathbf{K}$

$$\dot{\mathbf{K}} = 0, \tag{2.90}$$

where

$$\mathbf{K} = M\,\dot{\mathbf{R}} - \frac{q_R}{c}\,\mathbf{R} \times \mathbf{B} - \frac{q_{rR}}{c}\,\mathbf{r} \times \mathbf{B}. \tag{2.91}$$

The vector $\mathbf{K}$ is known as the total pseudomomentum [3]. We can rewrite Eq.(2.72) in terms of the total pseudomomentum

$$\mu\,\ddot{\mathbf{r}} = \frac{q_r}{c}\,\dot{\mathbf{r}} \times \mathbf{B} + \frac{q_{rR}}{Mc}\left(\mathbf{K} + \frac{q_R}{c}\,\mathbf{R} \times \mathbf{B} + \frac{q_{rR}}{c}\,\mathbf{r} \times \mathbf{B}\right) \times \mathbf{B} + \frac{q_1\,q_2}{|\mathbf{r}|^2}\hat{\mathbf{r}}. \tag{2.92}$$

If $q_R = 0$, Eq.(2.92) becomes

$$\mu\,\ddot{\mathbf{r}} = \frac{q_r}{c}\,\dot{\mathbf{r}} \times \mathbf{B} + \frac{q_{rR}}{Mc}\,\mathbf{K} \times \mathbf{B} + \frac{q_{rR}^2}{Mc^2}\,(\mathbf{r} \times \mathbf{B}) \times \mathbf{B} + \frac{q_1\,q_2}{|\mathbf{r}|^2}\hat{\mathbf{r}} \tag{2.93}$$

which can be rewritten using the vector identity $(\mathbf{A}\times\mathbf{B})\times\mathbf{C}=\mathbf{B}\,(\mathbf{A}\cdot\mathbf{C})-\mathbf{A}\,(\mathbf{B}\cdot\mathbf{C})$

$$\mu\,\ddot{\mathbf{r}}=\frac{q_r}{c}\,\dot{\mathbf{r}}\times\mathbf{B}+\frac{q_{rR}}{Mc}\,\mathbf{K}\times\mathbf{B}+\frac{q_{rR}^2}{Mc^2}\,\left(\mathbf{B}\,(\mathbf{r}\cdot\mathbf{B})-\mathbf{r}\mathbf{B}^2\right)+\frac{q_1\,q_2}{|\mathbf{r}|^2}\hat{\mathbf{r}}. \tag{2.94}$$

Eq.(2.94) only depends upon $\mathbf{R}$ implicitly through the pseudomomentum $\mathbf{K}$. In other words, if $q_R=0$ the motion of the relative-position vector is coupled to the center-of-mass vector by only a constant vector $\mathbf{K}$. This is known as the pseudoseparation of the relative position. Similarly using the total pseudomomentum, one can perform a pseudoseparation on the Hamiltonian. The pseudoseparation of the Hamiltonian can be used to analyze quantum atoms in the presence of a homogeneous magnetic field as long as the total charge of the system is zero [3].

Throughout the rest of this thesis we do not make use of the pseudomomentum or pseudoseparation. This has the advantage of allowing us to consider two-particle systems without specifying if $q_R=0$ or not. We also avoid the difficult task of trying to find a physical interpretation of the pseudomomentum [3].

2.7 Motion Boundedness

General analysis of motion in the z-direction is almost trivial since the B-field plays absolutely no role in the motion in the z-direction. The center-of-mass vector is always unbounded in the z-direction unless the initial velocity of the center-of-mass vector is zero. The relative-position vector is also unbounded unless the two particles' charges have opposite signs and the total z-component of angular momentum is small enough to lead to a bounded orbit. Therefore, in this section we will focus on the motion of particles in the xy-plane, that is to say motion perpendicular to the external magnetic field. The goal is to use the equations of motion and the initial conditions to determine if the motion of the center-of-mass $\mathbf{R}$ or the motion of the relative-position $\mathbf{r}$ is bounded in the xy-plane.

Let us begin by examining the motion of the center-of-mass vector under the assumption that we somehow already know that the relative-position vector is bounded. Later we shall consider the validity of the assumption that the relative-position vector is bounded. We are inspired to do this because numerical solutions show that the relative-position vector is bounded, and under this assumption we can greatly simplify Eq.(2.73). Now if $\mathbf{r}$ is bounded we can choose a time interval $t = [t_1, t_2]$ such that $|\dot{\mathbf{r}}_{avg}|$ is close to zero. Or, in more mathematical terms, we choose a $t = [t_1, t_2]$ such that $|\dot{\mathbf{r}}_{avg}| < \varepsilon$, where ε is arbitrarily small. And to be even more precise let us choose a $\triangle t = t_2 - t_1$ such that for any interval size $\triangle t$ we have $|\dot{\mathbf{r}}_{avg}| < \varepsilon$. To avoid taking the magnitude of all the equations of motion we define a vector $\mathbf{D}$ such that $|\mathbf{D}| = \varepsilon$ and $\mathbf{D}$ has the same direction of $\dot{\mathbf{r}}_{avg}$. Now we take the time average of Eq.(2.73) over $\triangle t$

$$\frac{1}{\triangle t}\int_{t_1}^{t_2} M\,\ddot{\mathbf{R}}dt = \frac{1}{\triangle t}\int_{t_1}^{t_2} \frac{q_R}{c}\,\dot{\mathbf{R}} \times \mathbf{B}dt + \frac{1}{\triangle t}\int_{t_1}^{t_2} \frac{q_{rR}}{c}\,\dot{\mathbf{r}} \times \mathbf{B}dt. \tag{2.95}$$

Because $\mathbf{B}$ is constant the second term on the righthand side of the equation is

$$\frac{1}{\triangle t}\int_{t_1}^{t_2} \frac{q_{rR}}{c}\,\dot{\mathbf{r}} \times \mathbf{B}dt = \frac{q_{rR}}{c}\frac{1}{\triangle t}\int_{t_1}^{t_2} \dot{\mathbf{r}}dt \times \mathbf{B} = \frac{q_{rR}}{c}\dot{\mathbf{r}}_{avg} \times \mathbf{B}. \tag{2.96}$$

The first term simplifies in a like matter. We use $|\dot{\mathbf{r}}_{avg}| < |\mathbf{D}|$ and the fact that $\mathbf{D}$ has the same direction as $\dot{\mathbf{r}}_{avg}$,

$$\frac{q_{rR}}{c}\dot{\mathbf{r}}_{avg} \times \mathbf{B} < \frac{q_{rR}}{c}\mathbf{D} \times \mathbf{B}. \tag{2.97}$$

We define a new vector $\mathbf{D}' = \frac{q_{rR}}{c}\mathbf{D} \times \mathbf{B}$. Furthermore we choose $\triangle t$ to be large enough that ε is so close to zero, that $\left|\mathbf{D}'\right|$ is also so close to zero that we can just assume it is zero. In other words, we choose $\triangle t$ so that

$$\left|\frac{q_{rR}}{c}\dot{\mathbf{r}}_{avg} \times \mathbf{B}\right| < \left|\mathbf{D}'\right| \approx 0. \tag{2.98}$$

Eq.(2.95) becomes

$$M\,\ddot{\mathbf{R}}_{avg} = \frac{q_R}{c}\,\dot{\mathbf{R}}_{avg} \times \mathbf{B}. \tag{2.99}$$

Eq.(2.99) is valid for all time intervals of size $\triangle t$. Let us make the equation continuous by looking at consecutive time intervals $[t_1, t_2]$, $[t_1 + \delta, t_2 + \delta]$, $[t_1 + 2\delta, t_2 + 2\delta]$, etc. where δ is small. These averages form a continuous function for $|\mathbf{R}_{avg}|(t)$ because $\mathbf{R}$, $\dot{\mathbf{R}}$, and $\ddot{\mathbf{R}}$ are all continuous. If q_R is not zero, Eq.(2.99) indicates that $\mathbf{R}_{avg}$ moves in a circle. The radius of the circle R is given by

$$R = \frac{M \left| \dot{\mathbf{R}}_{avg} \right|}{q_R B}. \tag{2.100}$$

Our analysis does not give $\left| \dot{\mathbf{R}}_{avg} \right|$ and therefore does not give R. However in certain cases one could, in theory, put an upper limit on $\dot{R}_{avg}$ by conservation of energy. In all cases $\dot{R}_{avg}$ is finite. And thus both $|\mathbf{R}_{avg}|$ and $|\mathbf{R}|$ are bounded. However if $q_R = 0$, that is to say if $q_1 = -q_2$, then we have

$$M \ddot{\mathbf{R}}_{avg} = 0, \tag{2.101}$$

$$\mathbf{R_{avg}} = \dot{\mathbf{R}}_{avg} t + \mathbf{R_o} \tag{2.102}$$

where $\mathbf{R_o}$ is a constant vector. In this special case, unless $\dot{\mathbf{R}}_{avg} = 0$, the motion of $\mathbf{R}_{avg}$ is unbounded and therefore $\mathbf{R}$ is also unbounded. Numerical experiments confirm these results (see section 2.8).

We now turn our attention to $\mathbf{r}$. If there is no magnetic field, the two particles are bounded to each other if and only if the electric force is attractive (the two charges have opposite signs) and the total energy of the system is negative (where the electric potential is set to be zero at infinity). Cases that are unbounded for opposite-sign charges with sufficient initial velocities occur because r becomes large enough so that there is negligible force on either particle. However with a magnetic field there is always a force on the two particles. Let us examine the contribution of this force. At large enough r the electric force term in Eq.(2.72) will vanish. The equations of

motion at large enough r become

$$\mu\,\ddot{\mathbf{r}} \approx \frac{q_r}{c}\,\dot{\mathbf{r}} \times \mathbf{B} + \frac{q_{rR}}{c}\,\dot{\mathbf{R}} \times \mathbf{B} \tag{2.103}$$

$$M\,\ddot{\mathbf{R}} = \frac{q_R}{c}\,\dot{\mathbf{R}} \times \mathbf{B} + \frac{q_{rR}}{c}\,\dot{\mathbf{r}} \times \mathbf{B}. \tag{2.104}$$

We argue that if for a given r the approximation that $\frac{q_1 q_2}{r} = 0$ in Eq.(2.103) is not good enough, we simply make r larger and Eq.(2.103) becomes an even better approximation. We also argue that we can continue to do this until the approximation is valid. However this author has no concrete analytic proof that this assumption is valid. Eq.(2.103) and Eq.(2.104) can be solved for exactly. The solutions in Cartesian coordinates are linear combinations of sine and cosine functions. However these solutions are lengthy and do not immediately reveal that $\mathbf{r}$ is bounded and therefore are not presented here. We are only interested in whether or not $\mathbf{r}$ is bounded, and we can prove this without writing down the solutions. We can rewrite Eq.(2.103) and Eq.(2.104) in terms of $\mathbf{r}_1$ and $\mathbf{r}_2$ yielding

$$m_1\,\ddot{\mathbf{r}}_1 = \frac{q_1}{c}\,\dot{\mathbf{r}}_\mathbf{1} \times \mathbf{B} \tag{2.105}$$

$$m_2\,\ddot{\mathbf{r}}_2 = \frac{q_2}{c}\,\dot{\mathbf{r}}_\mathbf{2} \times \mathbf{B}. \tag{2.106}$$

The solutions to Eq.(2.105) and Eq.(2.106) are circles whose radii and locations are determined by the initial conditions. Therefore the solution to $\mathbf{r}$ is simply the difference of the two circles, $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$, which means that $\mathbf{r}$ is bounded. If Eq.(2.103) is a valid approximation at large enough r, we have therefore shown that the assumption that we used to analyze the boundedness of $\mathbf{R}$, namely that $\mathbf{r}$ is always bounded is valid. Numerical solutions support these conclusions (see section 2.8).

2.8 Numerical Results

We were unable to obtain analytic solutions to Eq.(2.72) and Eq.(2.73); however we can obtain numerical solutions and examine the effects that a homogeneous magnetic field has on a classical two-particle system. These numerical solutions require that we specify mass and charge of each of the particles as well as their initial positions and velocities. In doing this we must be careful not to choose conditions that lead to a violation of the assumptions in Eq.(2.18), Eq.(2.21), and Eq.(2.26).

We are now ready to perform numerical simulations. In this section, we only look at motion in the xy-plane, or the plane perpendicular to the external magnetic field. The values for m_1, m_2, q_1, q_2, and B_o are not necessarily chosen to represent quantities that could easily be created in a lab. Instead, they are chosen, first, to ensure that the simulations are within the classical regime and, second, to highlight the importance of q_r, q_R, and q_{rR} in the equations. We want our simulations to satisfy Eq.(2.18); however, we do not know what a is for a given simulation. To get around this, we set the initial velocities of the two particles to be oppositely directed and perpendicular to the initial relative-position vectors. We then replace a with the initial relative-position distance in Eq.(2.18). We argue that the relative-position vector will be on the same order of magnitude as a. This assumption is not guaranteed to be correct, but for our simulations it works fine. We make no attempt to improve upon this crude estimation of a because Eq.(2.18) is already a rough approximation. For the first simulation we explicitly show that the assumptions in Eq.(2.18), Eq.(2.21), and Eq.(2.26) are satisfied. Subsequent simulations use similar values and explicit calculations of the assumptions are not presented.

2.8.1 First Simulation: $q_R = 0$

In this case, the equations of motion are

$$\mu\,\ddot{\mathbf{r}} = \frac{q_r}{c}\,\dot{\mathbf{r}} \times \mathbf{B} + \frac{q_{rR}}{c}\,\dot{\mathbf{R}} \times \mathbf{B} + \frac{q_1\,q_2}{|\mathbf{r}|^2}\hat{\mathbf{r}} \tag{2.107}$$

$$M\,\ddot{\mathbf{R}} = \frac{q_{rR}}{c}\,\dot{\mathbf{r}} \times \mathbf{B}. \tag{2.108}$$

We run our simulations with the following initial conditions

$$m_1 = 1\,kg \qquad m_2 = 2\,kg$$

$$q_1 = -1.055 * 10^{-5}\,C \qquad q_2 = 1.055 * 10^{-5}\,C$$

$$\mathbf{r}_1 = (-1.5, 0, 0)\ m \qquad \mathbf{r}_2 = (1.5, 0, 0)\ m$$

$$\dot{\mathbf{r}}_1 = (0, 0.25, 0)\ \frac{m}{s} \qquad \dot{\mathbf{r}}_2 = (0, -0.125, 0)\ \frac{m}{s}$$

$$B_o = 1000\,T.$$

We have written the initial conditions in SI units and we wish to see if they satisfy Eq.(2.18), Eq.(2.21), and Eq.(2.26) which are written for Gaussian units. This necessitates unit conversions. The details are omitted and only the results are shown in SI units.

We examine if these initial conditions satisfy Eq.(2.18) $GM \ll \frac{|q_1 q_2|}{\mu} \ll ac^2$. We have

$$GM \approx 2.00 * 10^{-11}\frac{m^3}{s^2} \ll \frac{|q_1 q_2|}{\mu} \approx 1.50\,\frac{m^3}{s^2} \ll ac^2 \approx 2.70 * 10^{17}\,\frac{m^3}{s^2},$$

meeting the criterion of Eq.(2.18).

We examine if these initial conditions satisfy Eq.(2.21) $PT = \frac{q^2 \ddot{r}^2_{avg}}{\pi c^3} T \ll \frac{1}{2} m v^2_{avg}$. We estimate the period T is 12 s from Fig 2.4. Again by using Fig 2.4, we estimate $\ddot{r}^2_{avg,1} \approx \left(\frac{1.25\,ms^{-1}}{6\,s}\right)^2 \approx .0434\ \frac{m^2}{s^4}$, and $\ddot{r}^2_{avg,2} \approx \left(\frac{0.7\,ms^{-1}}{6\,s}\right)^2 \approx .0136\ \frac{m^2}{s^4}$ for the average accelerations squared. Finally for the average squared velocities we will just use the

initial velocities. By Fig 2.4, we are underestimating the average squared velocities. This creates a stricter bound than if we had used the actual average squared velocities. Using these values we see that

$$\frac{2q_1^2\ddot{r}_{avg,1}^2}{3c^3}T \approx 1.43 * 10^{-36}\ J \ll \frac{1}{2}m_1 v_{avg}^2 \approx 0.03125\ J$$

and

$$\frac{2q_2^2\ddot{r}_{avg,2}^2}{3c^3}T \approx 4.50 * 10^{-37}\ J \ll \frac{1}{2}m_2 v_{avg}^2 \approx 0.01563\ J,$$

meeting the criterion of Eq.(2.21).

We examine if these initial conditions satisfy Eq.(2.26) which is $\sqrt{\frac{\mu|q_1 q_2|^2}{2\hbar^2|E|}} > 10^6$. The energy of the system is simply

$$E = \frac{1}{2}m_1 v_1^2 + \frac{1}{2}m_1 v_2^2 + V \approx -0.2865\ J$$

$$\sqrt{\frac{\mu\left|q_1 q_2\right|^2}{2\hbar^2\left|E\right|}} \approx 1.023 * 10^{34} \gg 10^6,$$

meeting the criterion of Eq.(2.26).

The simulations throughout the rest of this chapter use initial conditions of the same magnitude, and therefore all the simulations are considered to be in the classical regime.

Fig 2.1 shows that the two particles move in a bounded orbit when no magnetic field is present. Fig 2.2 shows the paths of the two particles in the presence of a magnetic field. Fig 2.3 shows the relative-position vector path as well as the center-of-mass vector path, and we can see that the relative-position vector path is bounded as predicted in Section 2.7. However, the center-of-mass vector is not bounded. Finally, Fig 2.4 shows the speeds of the two particles in that same field as a function of time, and one can observe that this graph is periodic.

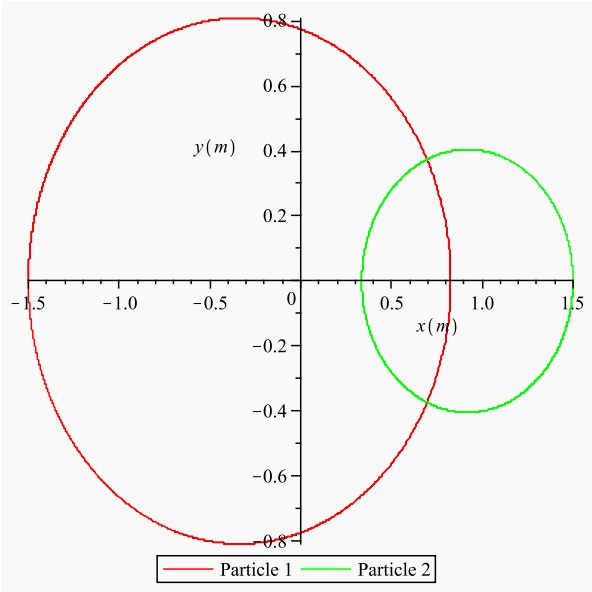

Figure 2.1 Particles move in bounded orbits when $B_o = 0$. This graph is the path of motion for $t = [0, 20]$ seconds.

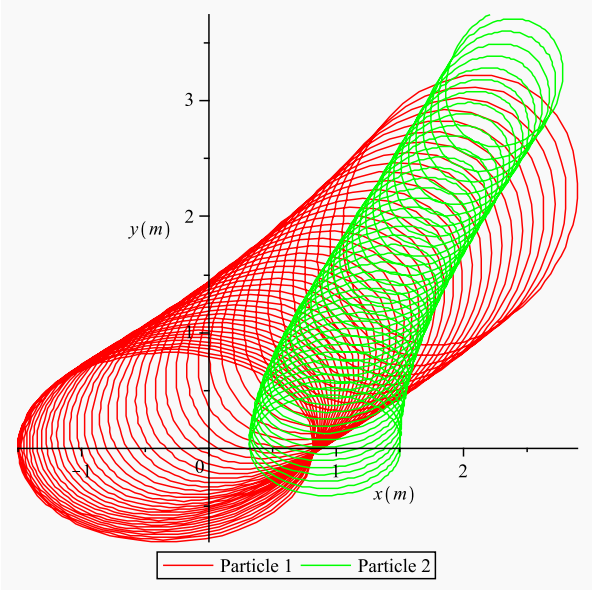

Figure 2.2 Particles paths of motion when $B_o = 1,000\,T$ for $t = [0, 500]$ seconds.

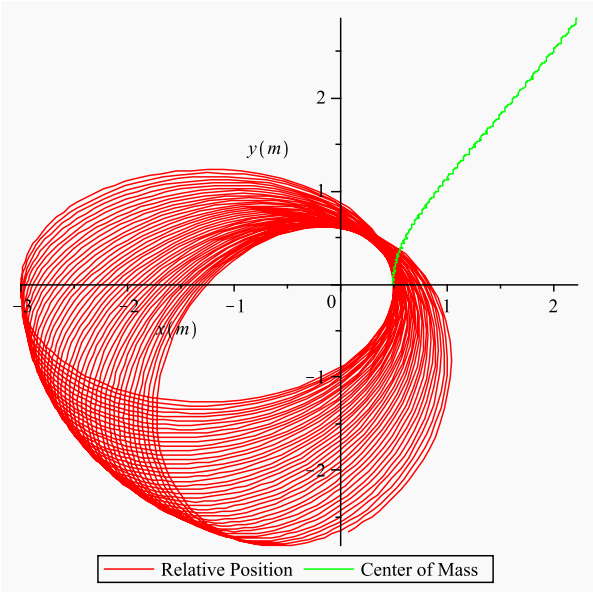

Figure 2.3 Relative-position and center-of-mass paths of motion when $B_o = 1,000\,T$ for $t = [0, 500]$ seconds.

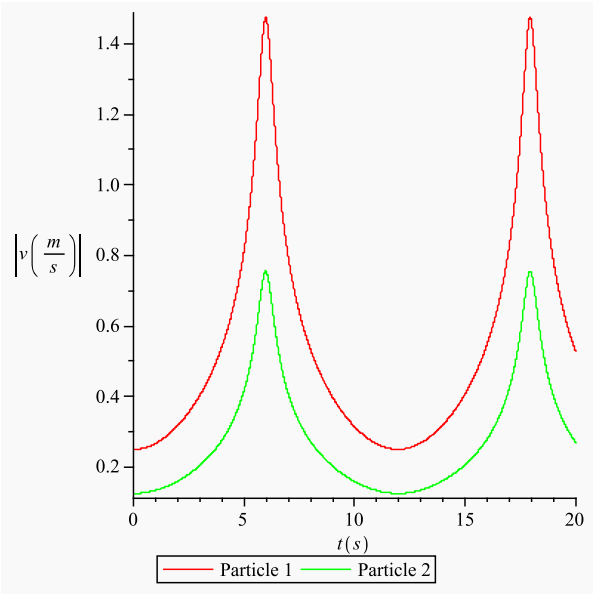

Figure 2.4 Speeds of particles one and two versus time when $B_o = 1,000\,T$ for $t = [0, 20]$ seconds.

2.8.2 Second Simulation: $q_r = 0$

In this case, the equations of motion are

$$\mu\,\ddot{\mathbf{r}} = \frac{q_{rR}}{c}\,\dot{\mathbf{R}} \times \mathbf{B} + \frac{q_1\,q_2}{|\mathbf{r}|^2}\hat{\mathbf{r}} \tag{2.109}$$

$$M\,\ddot{\mathbf{R}} = \frac{q_R}{c}\,\dot{\mathbf{R}} \times \mathbf{B} + \frac{q_{rR}}{c}\,\dot{\mathbf{r}} \times \mathbf{B}. \tag{2.110}$$

We run our simulations with the following initial conditions

$$m_1 = 1\,kg \qquad m_2 = 0.707\,kg$$

$$q_1 = -2.110 * 10^{-5}\,C \qquad q_2 = 1.055 * 10^{-5}\,C$$

$$\mathbf{r}_1 = (-1.5, 0, 0)\ m \qquad \mathbf{r}_2 = (1.5, 0, 0)\ m$$

$$\dot{\mathbf{r}}_1 = (0, 0.25, 0)\ \frac{m}{s} \qquad \dot{\mathbf{r}}_2 = (0, -0.354, 0)\ \frac{m}{s}$$

$$B_o = 100,000\,T.$$

These initial conditions are similar in magnitude to the first simulation except for B_o. By making B_o stronger for this simulation we can see the dramatic effect that the B-field has on the particles in the first period of motion. If we used a B-field strength similar to that of the first simulation the effect of the B-field would be slight.

These two particles would be in a bounded orbit without a magnetic field present. Fig 2.5 shows the paths of the two particles in the presence of a magnetic field. Fig 2.6 shows the relative-position vector path as well as the center-of-mass vector path, and we can see that the relative-position vector as well is the center-of-mass vector are bounded as predicted in section 2.7. Also, by Fig 2.6 we observe that both vectors are not perfectly periodic. They return close to their initial positions and begin the next period slightly out of phase with the first. Simulations over greater time periods not shown in this thesis reveal that the subsequent orbits will never be exactly in phase. Finally, Fig 2.7 shows the speeds of the two particles as a function of time.

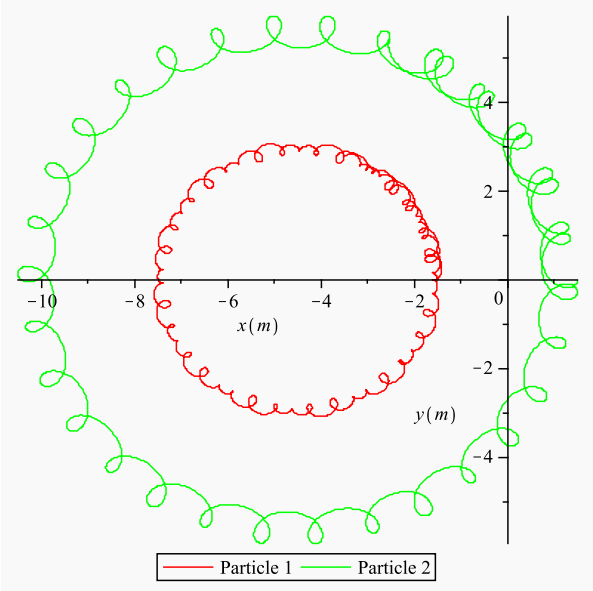

Figure 2.5 Particles paths of motion for $t = ([0, 154]$ seconds.

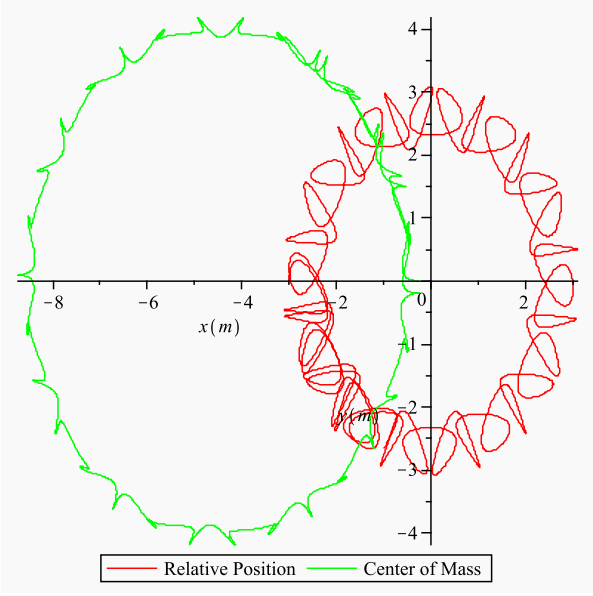

Figure 2.6 Relative-position and center-of-mass paths of motion for $t = [0, 154]$ seconds.

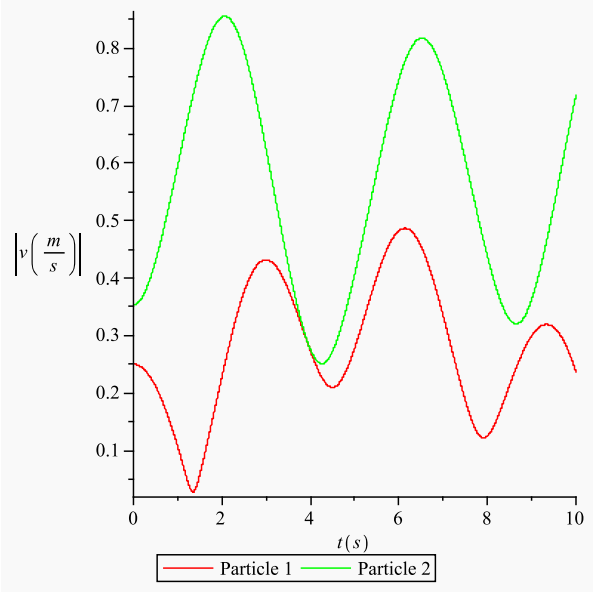

Figure 2.7 Speeds of particles one and two versus time for $t = [0, 10]$ seconds.

2.8.3 Third Simulation: $q_{rR} = 0$

In this case, the equations of motion are

$$\mu\,\ddot{\mathbf{r}} = \frac{q_r}{c}\,\dot{\mathbf{r}} \times \mathbf{B} + \frac{q_1\,q_2}{|\mathbf{r}|^2}\hat{\mathbf{r}} \tag{2.111}$$

$$M\,\ddot{\mathbf{R}} = \frac{q_R}{c}\,\dot{\mathbf{R}} \times \mathbf{B}. \tag{2.112}$$

We run our simulations with the following initial conditions

$$m_1 = 1\ kg \qquad m_2 = 1\ kg$$

$$q_1 = 1.055 * 10^{-5}\ C \qquad q_2 = 1.055 * 10^{-5}\ C$$

$$\mathbf{r}_1 = (-1.5, 0, 0)\ m \qquad \mathbf{r}_2 = (1.5, 0, 0)\ m$$

$$\dot{\mathbf{r}}_1 = (0, 0.01, 0)\ \frac{m}{s} \qquad \dot{\mathbf{r}}_2 = (0, -0.25, 0)\ \frac{m}{s}$$

$$B_o = 1000\ T.$$

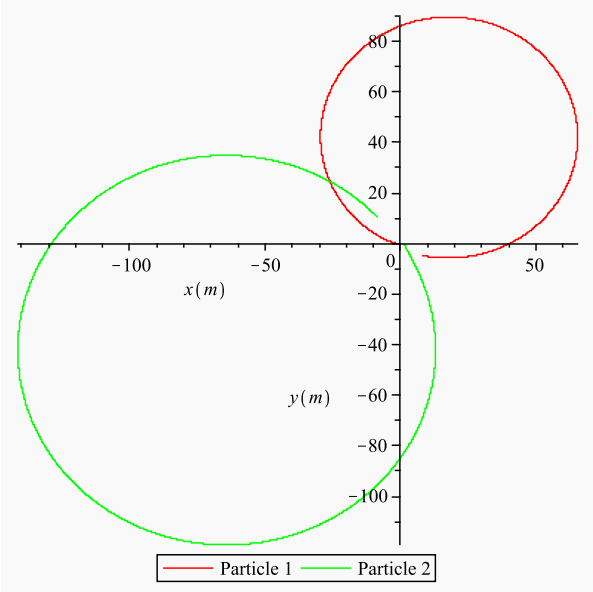

Figure 2.8 Particles paths of motion for $t = [0, 584]$ seconds.

These two particles repel one another and therefore would be unbounded without a magnetic field present. The magnetic field causes both particles to circle back towards one another as seen in Fig 2.8. As the particles approach each other, the electric repulsion between them deflects both of them as seen in Fig 2.9. After this both particles again circle back upon each other, but this time they have exchanged speeds as shown in Fig 2.12 and therefore the radii of the circles are also exchanged as seen in Fig 2.10. Fig 2.11 shows the relative-position vector path as well as the center-of-mass vector path, and we can see that the relative-position vector is bounded and the center-of-mass vector moves in a circle as predicted in section 2.7.

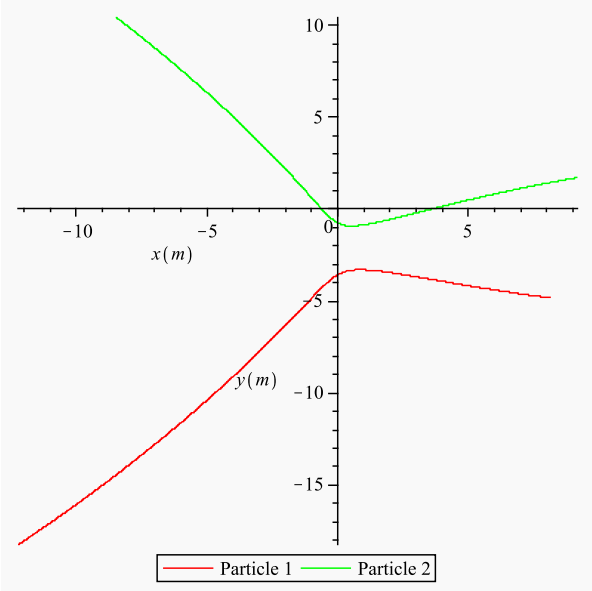

Figure 2.9 Particles paths of motion for $t = [584, 630]$ seconds.

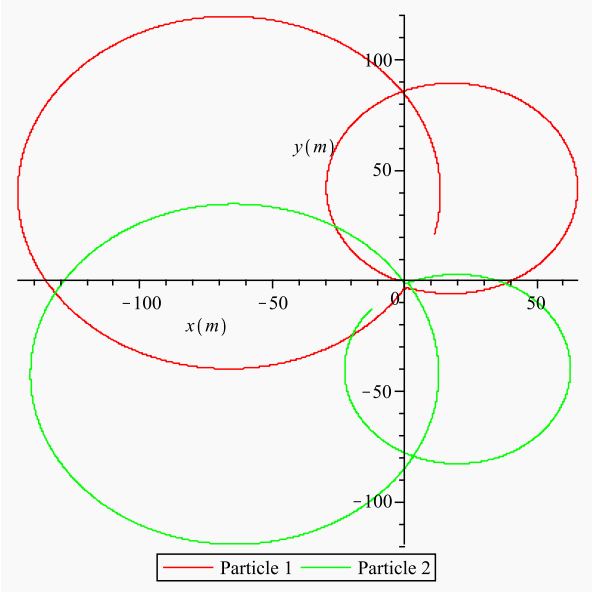

Figure 2.10 Particles paths of motion for $t = [0, 1173]$ seconds.

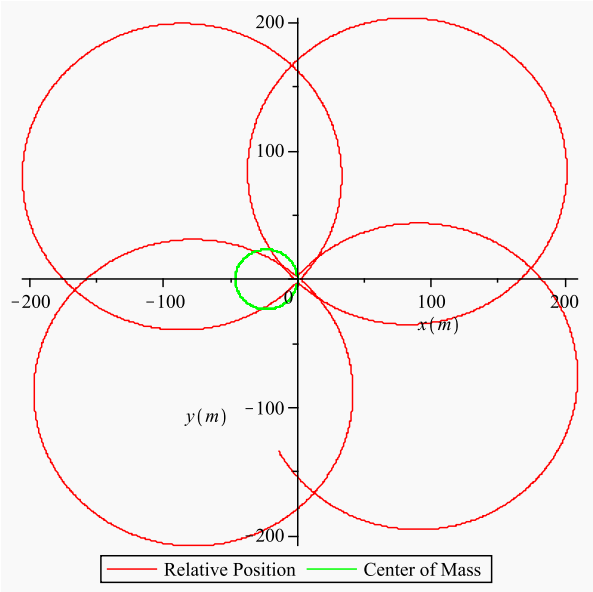

Figure 2.11 Relative-position and center-of-mass paths of motion for $t = [0, 2300]$ seconds.

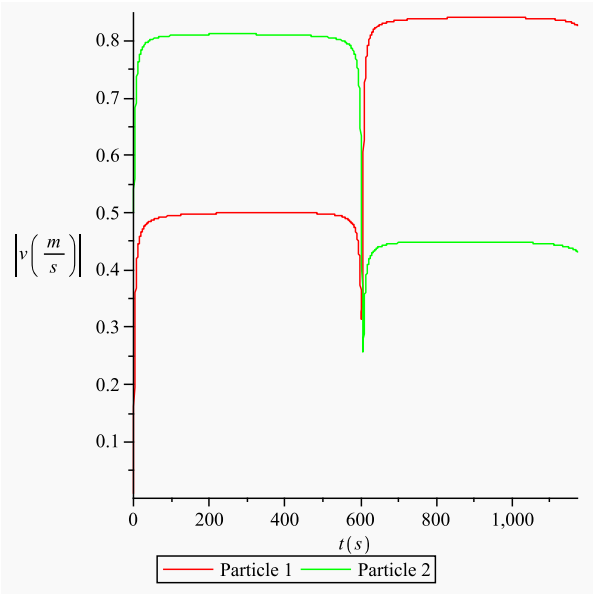

Figure 2.12 Speeds of particles one and two versus time for $t = [0, 1173]$ seconds.

2.8.4 Fourth Simulation: All Nonzero Charges

In this case, the equations of motion are Eq.(2.72) and Eq.(2.73). We run our simulations with the following initial conditions

$$m_1 = 1\,kg \qquad m_2 = 1.25\,kg$$

$$q_1 = 1.582 * 10^{-5}\,C \qquad q_2 = 1.055 * 10^{-5}\,C$$

$$\mathbf{r}_1 = (-1.5, 0, 0)\ m \qquad \mathbf{r}_2 = (1.5, 0, 0)\ m$$

$$\dot{\mathbf{r}}_1 = (0, 0.01, 0)\ \frac{m}{s} \qquad \dot{\mathbf{r}}_2 = (0, -0.5, 0)\ \frac{m}{s}$$

$$B_o = 10,000\,T$$

$$q_R = 2.637 * 10^{-5}\,C \qquad q_r = 6.967 * 10^{-6}\,C \qquad q_{rR} = 4.102 * 10^{-6}\,C.$$

When q_R, q_r, and q_{rR} are all nonzero, it is difficult to predict the resulting trajectories. We have done various simulations with all nonzero charges and we can only observe one common characteristic: in all the simulations the relative-position vector and the center-of-mass vector are bounded as predicted in section 2.7. In this thesis, we present one simulation where all the charges are nonzero.

Fig 2.14 shows that both the relative-position vector and the center-of-mass vector are bounded. Fig 2.13 shows that both particles move in near-circular paths indicating that the interaction with the magnetic field is more visible than the electrical interaction between the two particles. Fig 2.15 shows the velocities of the two particles.

We can see some common characteristics between this simulation and some of the previous simulations. For example, the wave nature of the two particles velocities in Fig 2.15 is similar to the wave nature of the velocities found in Fig 2.7 where $q_r = 0$. The sudden drop in velocities seen around $t = 175$ seconds in Fig 2.15 is similar to the one seen in Fig 2.12 where $q_{rR} = 0$ around $t = 600$ seconds.

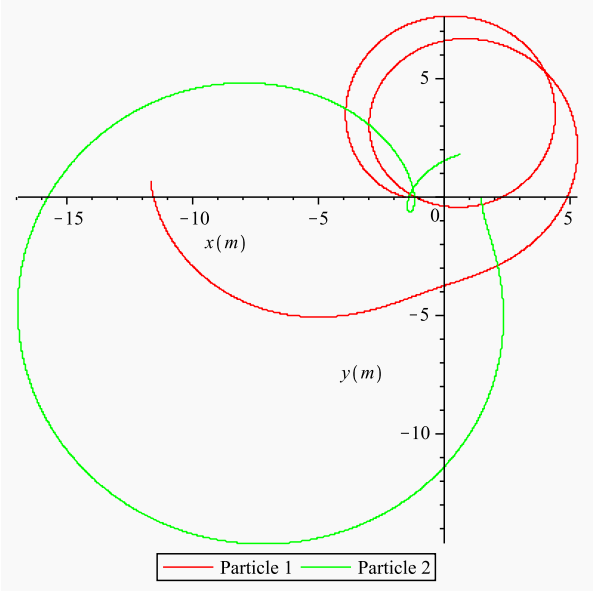

Figure 2.13 Particles paths of motion for $t = ([0, 100]$ seconds.

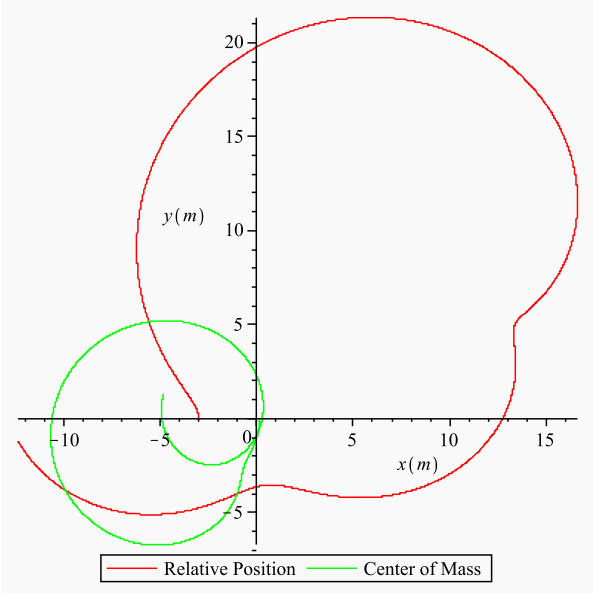

Figure 2.14 Relative-position and center-of-mass paths of motion for $t = [0, 100]$ seconds.

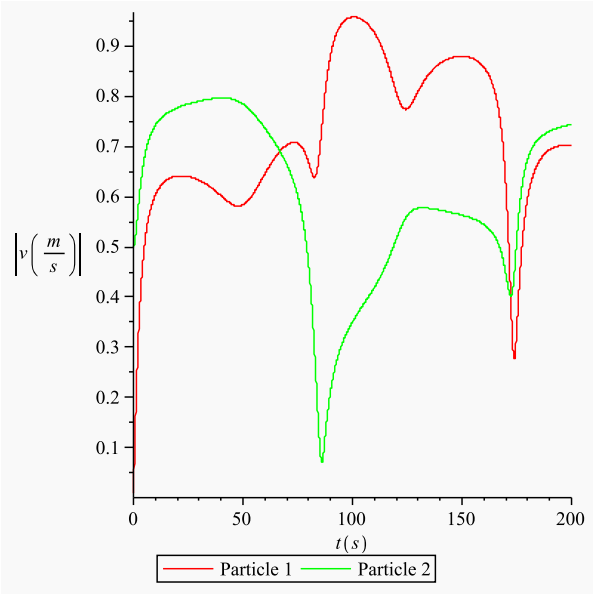

Figure 2.15 Speeds of particles one and two versus time for $t = [0, 200]$ seconds.

Chapter 3

Two Quantum Particles

3.1 Introduction

We examine the equations for two charged quantum particles in a homogeneous static magnetic field. We obtain the energy eigenvalues under the assumption of a weak magnetic field and compare them to those found in literature.

The Schrödinger-like equations we use in our analysis were first obtained by Reed and Brun [1]. The equations were obtained using a matrix factorization of the classical Hamiltonian which we discuss in Chapter 4. The classical Hamiltonian for N particles in an electromagnetic field is

$$H = \sum_{j=1}^{N} \left[\frac{1}{2m_j} \left(\mathbf{p}_j - \frac{q_j}{c} \mathbf{A}_j \right)^2 \right] + U, \tag{3.1}$$

where m_j, q_j, and $\mathbf{p}_j$ are respectively the mass, charge, and canonical momentum associated with the j^{th} particle, and U is the potential energy of the N particles due to external and interacting electric fields. Explicitly

$$U = U^{ext} + U^{int} = \sum_{j=1}^{N} q_j \phi \left(\mathbf{r}_j, t \right) + \sum_{j<k=1}^{N} \frac{q_j q_k}{|\mathbf{r}_j - \mathbf{r}_k|}, \tag{3.2}$$

where $\mathbf{r}_j$ is the position the j^{th} particle and $\phi(\mathbf{r}_j)$ is the scalar potential associated with the electromagnetic field at location $\mathbf{r}_j$. $\mathbf{A}_j$ is the vector potential associated with the j^{th} particle due to external magnetic fields and the interacting magnetic fields created by the motion of the other particles. Note that we have N different vector potentials, one associated with each particle, whereas we have only one scalar potential U. This happens because U enters the Hamiltonian as its own term whereas the vector potentials enter the Hamiltonian with the canonical momentum of each particle. We can write the vector potential to reflect the two sources

$$\mathbf{A}_j(\mathbf{r}_j) = \mathbf{A}^{ext}(\mathbf{r}_j) + \mathbf{A}_j^{int}(\mathbf{r}_j), \tag{3.3}$$

where $\mathbf{A}^{ext}$ is the vector potential of the external field and $\mathbf{A}_j^{int}$ is the vector potential due to the motion of the other particles. These vector potentials give the magnetic field acting on the j-particle

$$\mathbf{B}_j = \nabla \times \mathbf{A}_j = \nabla \times \mathbf{A}^{ext} + \nabla \times \mathbf{A}_j^{int}. \tag{3.4}$$

In Section 3.2 we begin by presenting the Schrödinger-like equations obtained by Reed and Brun [1] from the classical Hamiltonian in Eq.(3.1). We do not discuss the transition to the quantum (operator) Hamiltonian and the quantum states (wave functions). In essence the classical functions become quantum operators in the standard way. These operators act on the space of quantum states, which are multiple particle states obtained by using the tensor product of quantum states for individual particles. The spin terms appear as a result of the factorization (explained in Chapter 4) in analogy to the method used by Dirac in his work on the relativistic wave equation [9].

We seek to validate the matrix factorization method presented by Reed and Brun by applying the equations to analyze the Zeeman effect of two charged particles in an external magnetic field. In doing this we generalize the results of Reed and Brun by

keeping track of all the terms in the derivation and discussing the effects of neglecting some of these terms.

3.2 Wave Equations

The matrix factorization of Eq.(3.1) results in the following wave-spinor equation [1]

$$\left[\sum_{k=1}^{N}\frac{1}{2m_k}\left(\hat{\mathbf{p}}_k-\frac{q_k}{c}\hat{\mathbf{A}}_k\right)^2+U+\sum_{k=1}^{N}\frac{q_k\hbar}{2m_kc}\left(\hat{\sigma_k}\cdot\hat{\mathbf{B}}_j\right)\right]\chi=i\hbar\partial_t\chi, \tag{3.5}$$

where χ is the spinor that describes the spin-wave equations of N particles. If χ^j is the single spinor of the j^{th} particle then

$$\chi=\chi^1\otimes\chi^2...\otimes\chi^j...\otimes\chi^N \tag{3.6}$$

where $\otimes$ is the tensor (or Kronecker) product. The spin operator $\hat{\sigma}_j$ operates on the space of quantum states of the N particles and describes the spin of the j^{th} particle. In the Cartesian coordinate system (x,y,z) this is

$$\hat{\sigma}_j=[\sigma_{xj},\sigma_{yj},\sigma_{zj}] \tag{3.7}$$

where

$$\sigma_{xj}=I_{2^{j-1}}\otimes\sigma_x\otimes I_{2^{N-1}} \tag{3.8}$$

and σ_{yj} and σ_{zj} are defined similarly. I_k is the identity matrix of size $k\times k$. And σ_x, σ_y, and σ_z are the Pauli spin matrices

$$\sigma_x=\begin{bmatrix}0&1\\1&0\end{bmatrix},\ \sigma_y=\begin{bmatrix}0&-i\\i&0\end{bmatrix}\ \text{and}\ \sigma_z=\begin{bmatrix}1&0\\0&-1\end{bmatrix}. \tag{3.9}$$

The operators $\hat{\mathbf{p}}_j$, $\hat{\mathbf{A}}_j$ and $\hat{\mathbf{B}}_j$ are the momentum, vector potential, and magnetic field operators associated with the j^{th} particle

$$\hat{\mathbf{p}}_j=\frac{\hbar}{i}\nabla_j\ ,\ \hat{\mathbf{A}}_j=\mathbf{A}_j\left(\hat{\mathbf{r}}_j\right)\ \text{and}\ \hat{\mathbf{B}}_j=\nabla_j\times\hat{\mathbf{A}}_j=\mathbf{B}\left(\hat{\mathbf{r}}_j\right). \tag{3.10}$$

In this chapter we will only work with two particles without an external electric field and therefore Eq.(3.5) reduces to

$$\left[\frac{\left(\hat{\mathbf{p}}_1 - \frac{q_1}{c}\,\hat{\mathbf{A}}_1\right)^2}{2m_1} + \frac{\left(\hat{\mathbf{p}}_2 - \frac{q_2}{c}\,\hat{\mathbf{A}}_2\right)^2}{2m_2} + \right.$$

$$\left. \frac{q_1\, q_2}{|\hat{\mathbf{r}}_1 - \hat{\mathbf{r}}_2|} - \left(\frac{q_1\hbar}{2m_1 c}\hat{\sigma_1}\cdot\hat{\mathbf{B}}_1 + \frac{q_2\hbar}{2m_2 c}\hat{\sigma_2}\cdot\hat{\mathbf{B}}_2\right)\right]\chi = i\hbar\partial_t\chi. \quad (3.11)$$

Here χ is a 4×1 bi-spinor, and the spin operators $\hat{\sigma}_j$ are three 4×4 matrices.

3.3 Static Homogeneous Magnetic Field

Eq.(3.11) is greatly simplified under the assumption of a constant homogeneous magnetic field of magnitude B_o. As in Chapter 2 we will orient the z-axis along the B-field

$$\mathbf{B} = (0, 0, B_o)\,. \quad (3.12)$$

For the vector potential we choose the symmetric gauge

$$\mathbf{A}^{ext} = \frac{1}{2}B_o\ (-y, x, 0)\,. \quad (3.13)$$

We will assume that the internal magnetic fields due to the motion of the particles is negligible $\mathbf{A} = \mathbf{A}^{ext}$. Therefore the magnetic field is the same at any location and $\hat{\mathbf{B}}_1 = \hat{\mathbf{B}}_2$. Also $\hat{\sigma}_j\cdot\hat{\mathbf{B}} = \sigma_{zj}B_o$, since the B-field has only a z-component. The z-component of the particle spin matrices are 4×4 diagonal matrices,

$$\sigma_{z1} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix},\ \sigma_{z2} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}. \quad (3.14)$$

Therefore we can rewrite the terms with B_o in Eq.(3.11) as

$$\frac{\hbar B_o}{2c}\begin{bmatrix} \frac{q_1}{m_1}+\frac{q_2}{m_2} & 0 & 0 & 0 \\ 0 & -\frac{q_1}{m_1}+\frac{q_2}{m_2} & 0 & 0 \\ 0 & 0 & \frac{q_1}{m_1}-\frac{q_2}{m_2} & 0 \\ 0 & 0 & 0 & -\frac{q_1}{m_1}-\frac{q_2}{m_2} \end{bmatrix}\chi = \hat{\mathbf{S}}\chi. \tag{3.15}$$

This new operator $\hat{\mathbf{S}}$ has units of energy and measures the magnetic energy of a particular spin orientation. It represents the interaction energy of the combined spins with the external magnetic field.

We transform coordinates from particles one and two to the relative-position vector and center-of-mass vector as we did in Eq.(2.27), Eq.(2.29), and Eq.(2.30). We introduce the following new operators:

$$\hat{\mathbf{r}} = \hat{\mathbf{r}}_1 - \hat{\mathbf{r}}_2 = (\hat{x},\hat{y},\hat{z}) \quad \text{and} \quad \hat{\mathbf{R}} = \frac{m_1\hat{\mathbf{r}}_1 + m_2\hat{\mathbf{r}}_2}{m_1+m_2} = \left(\hat{X},\hat{Y},\hat{Z}\right), \tag{3.16}$$

$$\mu = \frac{m_1 m_2}{m_1+m_2} \quad , \quad M = m_1+m_2 \ , \tag{3.17}$$

$$\hat{\mathbf{p}} = \frac{m_2\hat{\mathbf{p}}_1 - m_1\hat{\mathbf{p}}_2}{m_1+m_2} = \frac{\hbar}{i}\nabla_{\mathbf{r}} \quad \text{and} \quad \hat{\mathbf{P}} = \hat{\mathbf{p}}_1+\hat{\mathbf{p}}_2 = \frac{\hbar}{i}\nabla_{\mathbf{R}}, \tag{3.18}$$

$$\hat{\mathbf{A}}_{\mathbf{r}} = \frac{1}{2}B_o\,(-\hat{y},\hat{x},0) \quad \text{and} \quad \hat{\mathbf{A}}_{\mathbf{R}} = \frac{1}{2}B_o\left(-\hat{Y},\hat{X},0\right). \tag{3.19}$$

And using the new charges introduced in Eq.(2.69)

$$q_r = \frac{m_2^2\,q_1 + m_1^2\,q_2}{M^2} \ , \ q_R = q_1+q_2 \ , \ q_{rR} = \frac{m_2\,q_1 - m_1\,q_2}{M} \tag{3.20}$$

Eq.(3.11) becomes

$$\left[\frac{\left(\hat{\mathbf{p}} - \frac{q_r}{c}\,\hat{\mathbf{A}}_{\mathbf{r}} - \frac{q_{rR}}{c}\,\hat{\mathbf{A}}_{\mathbf{R}}\right)^2}{2\mu} + \frac{\left(\hat{\mathbf{P}} - \frac{q_R}{c}\,\hat{\mathbf{A}}_{\mathbf{R}} - \frac{q_{rR}}{c}\,\hat{\mathbf{A}}_{\mathbf{r}}\right)^2}{2M} + \frac{q_1\,q_2}{|\hat{\mathbf{r}}_1-\hat{\mathbf{r}}_2|}\right]\chi = \left(\hat{E}+\hat{\mathbf{S}}\right)\chi \tag{3.21}$$

where $\hat{E} = i\hbar\partial_t$.

We can separate the operators on the left side of Eq.(3.21) into operators that operate on **r** only, operators that operate on **R** only, and operators that operate on both **r** and **R** with

$$\hat{H}_r = \frac{\left(\hat{\mathbf{p}} - \frac{q_r}{c}\hat{\mathbf{A}}_\mathbf{r}\right)^2}{2\mu} + \frac{q_1\, q_2}{|\mathbf{r}|}, \tag{3.22}$$

$$\hat{H}_R = \frac{\left(\hat{\mathbf{P}} - \frac{q_R}{c}\hat{\mathbf{A}}_\mathbf{R}\right)^2}{2M}, \tag{3.23}$$

and

$$\hat{H}_{rR} = -\frac{q_{rR}}{c}\left(\frac{1}{\mu}\hat{\mathbf{A}}_\mathbf{R}\hat{\mathbf{p}} + \frac{1}{M}\hat{\mathbf{A}}_\mathbf{r}\hat{\mathbf{P}}\right) + \frac{q_{rR}^2}{c^2}\left[\left(\frac{1}{M}+\frac{1}{\mu}\right)\hat{\mathbf{A}}_\mathbf{R}\hat{\mathbf{A}}\mathbf{r} + \frac{1}{2\mu}\hat{\mathbf{A}}_\mathbf{R}^2 + \frac{1}{2M}\hat{\mathbf{A}}_\mathbf{r}^2\right]. \tag{3.24}$$

Eq.(3.21) becomes

$$\left(\hat{H}_r + \hat{H}_R + \hat{H}_{rR}\right)\chi = \left(\hat{E} + \hat{\mathbf{S}}\right)\chi. \tag{3.25}$$

We can use separation of variables to solve for the time portion of χ. We let

$$\chi = \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix} = \begin{bmatrix} f_1(t)\, g_1(\mathbf{r},\mathbf{R}) \\ f_2(t)\, g_2(\mathbf{r},\mathbf{R}) \\ f_3(t)\, g_3(\mathbf{r},\mathbf{R}) \\ f_4(t)\, g_4(\mathbf{r},\mathbf{R}) \end{bmatrix}. \tag{3.26}$$

Substituting this in Eq.(3.25) and rearranging terms yields four equations

$$\frac{\left(\hat{H}_r + \hat{H}_R + \hat{H}_{rR} - \hat{\mathbf{S}}_{jj}\right) g_j}{g_j} = \frac{\hat{E} f_j}{f_j}. \tag{3.27}$$

The right hand side of Eq.(3.27) is time dependent only and the left hand side has no time dependence; therefore both sides must be equal to a constant E^{tot}, which apparently is the total energy of the two-particle system.

$$f_j(t) = e^{-\frac{i}{\hbar}E_j^{tot}t}. \tag{3.28}$$

In general, we cannot use separation of variables to separate the $\mathbf{r}$ and $\mathbf{R}$ dependence of g_j because $\hat{H}_{rR}$ operates on both terms. This is analogous to the classic case where we found that the equations of motion Eq.(2.72) and Eq.(2.73) were coupled. In order to obtain some solution we will treat $\hat{H}_{rR}$ as a perturbation. To lowest order we expect to obtain accurate eigenstate energies, but not necessarily accurate wave functions.

Treating $\hat{H}_{rR}$ as a perturbation allows us to write g_j as a product of two functions one of $\mathbf{r}$, $k_j(\mathbf{r})$, and one of $\mathbf{R}$, $l_j(\mathbf{R})$, and then use separation of variables. We obtain the following two spinor equations

$$\hat{H}_r k_j = E_j^{\mathbf{r}} k_j + \hat{S}_{jj} k_j, \tag{3.29}$$

$$\hat{H}_R l_j = E_j^{\mathbf{R}} l_j \tag{3.30}$$

where $E_j^{\mathbf{r}}$ and $E_j^{\mathbf{R}}$ are constants and $E_j^{tot} = E_j^{\mathbf{r}} + E_j^{\mathbf{R}}$. First we look at Eq.(3.29) in more detail,

$$\left[\frac{\left(\hat{\mathbf{p}} - \frac{q_r}{c} \hat{\mathbf{A}}_{\mathbf{r}} \right)^2}{2\mu} + \frac{q_1 \, q_2}{|\mathbf{r}|} \right] k_j = E_j^{\mathbf{r}} k_j + \hat{S}_{jj} k_j. \tag{3.31}$$

We can obtain a solution if we treat the $\hat{\mathbf{A}}_{\mathbf{r}}^2$ term as a perturbation. This is reasonable if the magnetic field is weak

$$\frac{\left(\hat{\mathbf{p}} - \frac{q_r}{c} \hat{\mathbf{A}}_{\mathbf{r}} \right)^2}{2\mu} \approx \frac{\hat{\mathbf{p}}^2 - 2\frac{q_r}{c} \hat{\mathbf{A}}_{\mathbf{r}} \cdot \hat{\mathbf{p}}}{2\mu}. \tag{3.32}$$

Next, observe that

$$\hat{\mathbf{A}}_{\mathbf{r}} \cdot \hat{\mathbf{p}} = i\hbar \frac{B_o}{2} \left(y \frac{\partial}{\partial x} - x \frac{\partial}{\partial y} \right) = \frac{B_o}{2} \hat{L}_z \tag{3.33}$$

where $\hat{L}_z$ is the z-component of the angular momentum operator. Eq.(3.29) becomes

$$\left[\frac{\hat{\mathbf{p}}^2 - \frac{q_r}{c} B_o \hat{L}_z}{2\mu} + \frac{q_1 \, q_2}{|\mathbf{r}|} \right] k_j = E_j^{\mathbf{r}} k_j + \hat{S}_{jj} k_j. \tag{3.34}$$

We can obtain a solution for the specific case when $q_1\, q_2 < 0$. When $q_1\, q_2 < 0$ and $B_o = 0$, Eq.(3.34) reduces to the wave equation of an electron of a hydrogen atom with a mass μ. This wave equation has the known hydrogen eigensolutions ψ_{nlm}, where n is associated with the energy level, l is associated with the angular momentum, and m is associated with the z-component of angular momentum. We note that ψ_{nlm} is also an eigenfunction of $\hat{L}_z$. When $q_1\, q_2 < 0$ and $B_o \neq 0$ we get the spinor solution and energy splitting,

$$k_j\left(\mathbf{r}\right) = \psi_{nlm}\left(\mathbf{r}\right) \tag{3.35}$$

for all j

$$\left(\left[\frac{\hat{\mathbf{p}}^2 - \frac{q_r}{c}\, B_o \hat{L}_z}{2\mu} + \frac{q_1\, q_2}{|\mathbf{r}|}\right]\psi_{nlm}\right)/\psi_{nlm} - \hat{S}_{jj} = E_j^{\mathbf{r}}. \tag{3.36}$$

Note

$$\left(\left[\frac{\hat{\mathbf{p}}^2 - \frac{q_r}{c}\, B_o \hat{L}_z}{2\mu} + \frac{q_1\, q_2}{|\mathbf{r}|}\right]\psi_{nlm}\right)/\psi_{nlm} = E_{nlm}^{j} - \frac{\hbar m B_o q_r}{2c\mu}. \tag{3.37}$$

The four energy levels are therefore,

$$E_{nlm} - \frac{\hbar B_o}{2c}\left(\frac{m q_r}{\mu} + \begin{bmatrix} \frac{q_1}{m_1} + \frac{q_2}{m_2} \\ -\frac{q_1}{m_1} + \frac{q_2}{m_2} \\ \frac{q_1}{m_1} - \frac{q_2}{m_2} \\ -\frac{q_1}{m_1} - \frac{q_2}{m_2} \end{bmatrix}\right). \tag{3.38}$$

If we assume that $q_2 = -q_1$, or in other words the system is neutral, the energy levels are

$$E_{nlm} - \frac{\hbar B_o q_1}{2c}\left(\frac{m}{m_1} - \frac{m}{m_2} + \begin{bmatrix} \frac{1}{m_1} - \frac{1}{m_2} \\ -\frac{1}{m_1} - \frac{1}{m_2} \\ \frac{1}{m_1} + \frac{1}{m_2} \\ -\frac{1}{m_1} + \frac{1}{m_2} \end{bmatrix}\right), \tag{3.39}$$

$$E_{nlm} - \frac{\hbar B_o q_1}{2c} \begin{bmatrix} \left(\frac{1}{m_1} - \frac{1}{m_2}\right)(m+1) \\ \frac{m-1}{m_1} - \frac{m+1}{m_2} \\ \frac{m+1}{m_1} - \frac{m-1}{m_2} \\ \left(\frac{1}{m_1} - \frac{1}{m_2}\right)(m-1) \end{bmatrix}. \tag{3.40}$$

Next, we look at the center-of-mass equation Eq.(3.30). Assuming $q_R \neq 0$, this is Schrödinger's equation of a charged particle of mass M and charge q_R in a uniform magnetic field and is known as the Landau problem. We now switch to a new vector potential for $\hat{A}_{\mathbf{R}}$, which represents the same magnetic field

$$\hat{A}_{\mathbf{R}} = B_o \left(0, \hat{X}, 0\right). \tag{3.41}$$

The solution to the Landau problem with this vector potential can be found in Phillip Du Toit's Senior Thesis, Appendix E [10]. The eigenstate solutions for all j are

$$l_j(\mathbf{R}) = l_{\eta,k_y,k_z}(X,Y,Z) = \left(\frac{M\omega_c}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^\eta \eta!}} H_\eta(\xi) e^{-\frac{\xi^2}{2} + ik_y Y + ik_z Z}, \tag{3.42}$$

where

$$\omega_c = \frac{q_R B_0}{cM} \qquad \xi = \sqrt{\frac{M\omega_c}{\hbar}}(X - X_0) \qquad X_0 = \frac{\hbar k_y c}{q_R B_0}. \tag{3.43}$$

H_η are Hermite polynomials. The eigenstate energies are,

$$E_{\eta,k_z} = (\eta + \frac{1}{2})\hbar\,|\omega_c| + E_z \tag{3.44}$$

$$E_{\eta,k_z} = (\eta + \frac{1}{2})\hbar\,|\omega_c| + \frac{\hbar^2}{2M}k_z^2. \tag{3.45}$$

If $q_R = 0$, then $\hat{H}_R = 0$ and $l_j(\mathbf{R})$ is the wave solution of a free particle of mass M for all j.

3.4 First Energy Corrections Due to Perturbations

In order to get an analytical solution of Eq.(3.21) we treated the following terms as perturbations

$$\hat{H}_p = \hat{H}_{rR} + \frac{q_r^2}{2c^2\mu}\hat{\mathbf{A}}_{\mathbf{r}}^2 \tag{3.46}$$

with

$$\hat{H}_{rR} = -\frac{q_{rR}}{c}\left(\frac{1}{\mu}\hat{\mathbf{A}}_{\mathbf{R}}\hat{\mathbf{p}} + \frac{1}{M}\hat{\mathbf{A}}_{\mathbf{r}}\hat{\mathbf{P}}\right) + \frac{q_{rR}^2}{c^2}\left[\left(\frac{1}{M}+\frac{1}{\mu}\right)\hat{\mathbf{A}}_{\mathbf{R}}\hat{\mathbf{A}}\mathbf{r} + \frac{1}{2\mu}\hat{\mathbf{A}}_{\mathbf{R}}^2 + \frac{1}{2M}\hat{\mathbf{A}}_{\mathbf{r}}^2\right]. \tag{3.47}$$

Using nondegenerate quantum perturbation theory, the first-order energy correction is

$$E^{(1)} = \langle l_j(\mathbf{R})\, k_j(\mathbf{r}) \mid \hat{H}_p \mid l_j(\mathbf{R})\, k_j(\mathbf{r})\rangle. \tag{3.48}$$

We will evaluate $E^{(1)}$ term by term. We can factorize the terms based on what operates on $\mathbf{R}$ and what operates on $\mathbf{r}$. For example,

$$\langle l_j(\mathbf{R})\, k_j(\mathbf{r}) \mid \hat{\mathbf{A}}_{\mathbf{R}}\hat{\mathbf{p}} \mid l_j(\mathbf{R})\, k_j(\mathbf{r})\rangle = \langle l_j(\mathbf{R}) \mid \hat{\mathbf{A}}_{\mathbf{R}} \mid l_j(\mathbf{R})\rangle \cdot \langle k_j(\mathbf{r}) \mid \hat{\mathbf{p}} \mid k_j(\mathbf{r})\rangle. \tag{3.49}$$

We then observe that some of these factors terms are zero. For example,

$$\langle k_j(\mathbf{r}) \mid \hat{\mathbf{p}} \mid k_j(\mathbf{r})\rangle = 0 \tag{3.50}$$

because by symmetry the expected momentum for the wave function of a hydrogen atom is zero. We also note that due to parity ($\mathbf{r} \to -\mathbf{r}$)

$$\langle k_j(\mathbf{r}) \mid \hat{\mathbf{A}}_{\mathbf{r}} \mid k_j(\mathbf{r})\rangle = \frac{B_o}{2}\left(-\langle k_j(\mathbf{r}) \mid \hat{y} \mid k_j(\mathbf{r})\rangle, \langle k_j(\mathbf{r}) \mid \hat{x} \mid k_j(\mathbf{r})\rangle, 0\right) = 0. \tag{3.51}$$

Therefore by Eq.(3.51) and Eq.(3.50), we see that

$$\langle l_j(\mathbf{R})\, k_j(\mathbf{r}) \mid \hat{\mathbf{A}}_{\mathbf{R}}\hat{\mathbf{p}} \mid l_j(\mathbf{R})\, k_j(\mathbf{r})\rangle = 0, \tag{3.52}$$

$$\langle l_j(\mathbf{R})\, k_j(\mathbf{r}) \mid \hat{\mathbf{A}}_{\mathbf{r}}\hat{\mathbf{P}} \mid l_j(\mathbf{R})\, k_j(\mathbf{r})\rangle = 0, \tag{3.53}$$

$$\langle l_j(\mathbf{R})\, k_j(\mathbf{r}) \mid \hat{\mathbf{A}}_\mathbf{r}\hat{\mathbf{A}}_\mathbf{R} \mid l_j(\mathbf{R})\, k_j(\mathbf{r})\rangle = 0. \tag{3.54}$$

The nonzero terms of $\hat{H}_p$ for the first-order energy correction are

$$\hat{H}_p^{(1)} = \frac{q_{rR}^2}{2c^2}\left[\frac{1}{\mu}\hat{\mathbf{A}}_\mathbf{R}^2 + \frac{1}{M}\hat{\mathbf{A}}_\mathbf{r}^2\right] + \frac{q_r^2}{2c^2\mu}\hat{\mathbf{A}}_\mathbf{r}^2. \tag{3.55}$$

3.4.1 The $\hat{\mathbf{A}}_\mathbf{R}^2$ Term

For the first nonzero term of the energy correction we need to evaluate

$$\langle l_j(\mathbf{R}) \mid \hat{\mathbf{A}}_\mathbf{R}^2 \mid l_j(\mathbf{R})\rangle = B_o^2\langle l_j(\mathbf{R}) \mid \hat{X}^2 \mid l_j(\mathbf{R})\rangle. \tag{3.56}$$

In evaluating the above integral, the factors containing the Y and Z components disappear[1] and the integral becomes

$$\langle \varphi_\eta(X - X_o) \mid \hat{X}^2 \mid \varphi_\eta(X - X_o)\rangle = \langle \varphi_\eta(X) \mid \hat{X}^2 \mid \varphi_\eta(X)\rangle + X_o^2 \tag{3.57}$$

where $\varphi_\eta(X)$ are the quantum eigenfunctions for the simple harmonic oscillator. The expected X^2 values are obtained from the expected potential energy $\langle\hat{V}\rangle$ found in [11] using the fact that $\hat{V} = \frac{1}{2}M\omega_c^2\hat{X}^2$

$$\langle \varphi_\eta(X) \mid \hat{X}^2 \mid \varphi_\eta(X)\rangle = \frac{\hbar(2\eta+1)}{2M\omega_c}. \tag{3.58}$$

Therefore,

$$\langle l_j(\mathbf{R}) \mid \frac{q_{rR}^2}{2\mu c^2}\hat{\mathbf{A}}_\mathbf{R}^2 \mid l_j(\mathbf{R})\rangle = \frac{B_o\hbar q_{rR}^2}{4q_R c\mu}(2\eta+1) + \frac{q_{rR}^2\hbar^2k_y^2}{2q_R^2\mu}. \tag{3.59}$$

The perturbation we evaluated above is proportional to B_o^2, however, the first-order energy correction contains a term that does not contain B_o but instead contains k_y^2. It is difficult to interpret this term since k_y is independent of energy and can be any real number. It is an artifact of our perturbation analysis, and we can eliminate it by not

[1] To avoid singularities, we integrate over a finite box of length L in both directions Y and Z and we take the limit $L \to \infty$ after the integration.

treating the $\frac{q_{rR}^2}{2\mu c^2}\hat{\mathbf{A}}_{\mathbf{R}}^2$ as a perturbation but as part of $\hat{H}_R$. We define $\hat{H}'_R = \hat{H}_R + \frac{q_{rR}^2}{2\mu c^2}\hat{\mathbf{A}}_{\mathbf{R}}^2$ and we also go back to our original gauge potential

$$\hat{\mathbf{A}}_{\mathbf{R}} = \frac{1}{2}B_o\left(-\hat{Y}, \hat{X}, 0\right).$$

We do this to make the Hamiltonian $\hat{H}'_R$ similar to a Hamiltonian that has known, exact solutions. The Hamiltonian that has known, exact solutions, $\hat{H}_q$, is the Hamiltonian of a charged particle in a uniform magnetic field and an isotropic oscillator.

$$\hat{H}_q = \frac{\hat{\mathbf{p}}}{2m} + \frac{m\omega_o\hat{\mathbf{r}}^2}{2} - \frac{q\hat{\mathbf{A}}\cdot\hat{\mathbf{p}}}{mc} + \frac{q^2\hat{\mathbf{A}}^2}{2mc^2} \tag{3.60}$$

$$\hat{H}'_R = \frac{\hat{\mathbf{P}}}{2M} + \frac{q_{rR}^2B_o^2}{8\mu c}\left(\hat{X}^2 + \hat{Y}^2\right) - \frac{q_{rR}\hat{\mathbf{A}}_{\mathbf{R}}\cdot\hat{\mathbf{P}}}{Mc} + \frac{q_{rR}^2\hat{\mathbf{A}}_{\mathbf{R}}^2}{2Mc^2} \tag{3.61}$$

If one is to set $\omega_o = \frac{q_{rR}B_o}{2c\sqrt{M\mu}}$ and only look at the operators that operate on X and Y, the two Hamiltonians are identical. Since we are mainly interested in eigenstate energies we will not present the exact eigenfunction solutions of $\hat{H}'_R$; however the eigenstate energies are easily obtained by examining the eigenstate energies of $\hat{H}_q^{\perp}$, where $\perp$ refers to the Hamiltonian components perpendicular to the B-field or the x and y components, which can be found in [12]

$$E_q^{\perp} = \hbar\omega\left(\eta_r + \eta_l + 1\right) - \frac{\hbar\omega_c}{2}\left(\eta_r - \eta_l\right), \tag{3.62}$$

where $\omega = \sqrt{\omega_o^2 + \frac{\omega_c^2}{4}}$ and ω_c is given by Eq.(3.43). For our problem we have

$$E_{\eta_r,\eta_l,k_z} = \frac{\hbar B_o}{2cM}\left(\sqrt{\frac{q_{rR}^2M}{\mu} + q_R^2}\left(\eta_r + \eta_l + 1\right) + q_R\left(n_l - n_r\right)\right) + \frac{\hbar^2}{2M}k_z^2. \tag{3.63}$$

Notice if we set $q_{rR} = 0$ we recover Eq.(3.45) where $\eta = \eta_l$ if $q_R > 0$ and $\eta = \eta_r$ if $q_R < 0$. η_l is the quantum number of left-circular polarized quanta and η_r is the quantum number of right-circular polarized quanta. Our original solution given by Eq.(3.45) only contained one quantum number which was either η_l or η_r. Classically

we can view this as a charged particle in a uniform magnetic field. Depending on its charge, the particle will either travel counter-clockwise or clockwise when looking against the B-field in the plane perpendicular to the B-field. Therefore we need only one quantum number η_l or η_r to describe the energy levels. However, we introduced a new term with charge q_{rR}, and since q_{rR} and q_R do not have to have the same sign it becomes necessary to introduce both quantum numbers η_l and η_r. Had we chosen a different set of eigenfunctions that used two quantum numbers η_l and η_r of the original Hamiltonian $\hat{H}_R$ (this can be accomplished using a different gauge then the one chosen in the text) and then done perturbation analysis, I suspect that we would not have obtained an artifact term like the term with k_y^2 obtained in Eq.(3.59). However, since we were able to find the exact energy eigenstates without perturbation analysis, we will not attempt to do this.

3.4.2 The $\hat{\mathbf{A}}_{\mathbf{r}}^2$ Terms

We are left with the following Hamiltonian to evaluate:

$$H_l = \frac{q_{rR}^2}{2Mc^2}\hat{\mathbf{A}}_{\mathbf{r}}^2 + \frac{q_r^2}{2c^2\mu}\hat{\mathbf{A}}_{\mathbf{r}}^2. \tag{3.64}$$

Eq.(3.64) is first evaluated using Maple© (see Appendix B). Fig 3.1 list the first-order energy corrections for $n = 1, 2, 3$ for all possible l and m values. In the table we use a, the Bohr radius of the hydrogen-like atom, where

$$a = \frac{\hbar^2}{\mu\,|q_1 q_2|}. \tag{3.65}$$

We can also find analytical expressions for the perturbation terms in Eq.(3.64) for an arbitrary n, l, and m. Both terms require us to calculate the following integral when working in the symmetric gauge

n	l	m	$E^{(1)}$
1	0	0	$\frac{a^2B_o^2}{4c^2}\left(\frac{q_r^2}{\mu}+\frac{q_{rR}^2}{M}\right)$
2	0	0	$\frac{7a^2B_o^2}{2c^2}\left(\frac{q_r^2}{\mu}+\frac{q_{rR}^2}{M}\right)$
2	1	0	$\frac{3a^2B_o^2}{2c^2}\left(\frac{q_r^2}{\mu}+\frac{q_{rR}^2}{M}\right)$
2	1	±1	$3\frac{a^2B_o^2}{c^2}\left(\frac{q_r^2}{\mu}+\frac{q_{rR}^2}{M}\right)$
3	0	0	$\frac{69a^2B_o^2}{4c^2}\left(\frac{q_r^2}{\mu}+\frac{q_{rR}^2}{M}\right)$
3	1	0	$9\frac{a^2B_o^2}{c^2}\left(\frac{q_r^2}{\mu}+\frac{q_{rR}^2}{M}\right)$
3	1	±1	$18\frac{a^2B_o^2}{c^2}\left(\frac{q_r^2}{\mu}+\frac{q_{rR}^2}{M}\right)$
3	2	0	$\frac{15a^2B_o^2}{2c^2}\left(\frac{q_r^2}{\mu}+\frac{q_{rR}^2}{M}\right)$
3	2	±1	$9\frac{a^2B_o^2}{c^2}\left(\frac{q_r^2}{\mu}+\frac{q_{rR}^2}{M}\right)$
3	2	±2	$\frac{27a^2B_o^2}{2c^2}\left(\frac{q_r^2}{\mu}+\frac{q_{rR}^2}{M}\right)$

Figure 3.1 Table of first-order energy corrections.

$$\langle \psi_{nlm}(\mathbf{r}) \mid \hat{x}^2 + \hat{y}^2 \mid \psi_{nlm}(\mathbf{r}) \rangle = \langle R_{nl}(r) Y_{lm}(\theta,\phi) \mid r^2 \sin^2(\theta) \mid R_{nl}(r) Y_{lm}(\theta,\phi) \rangle, \tag{3.66}$$

where R_{nl} is the radial part of the wave solutions of hydrogen and Y_{lm} are spherical harmonics. Note that $\psi_{nlm} = R_{nl} Y_{lm}$.

We break the integral into two factors

$$\langle R_{nl}(r) Y_{lm}(\theta,\phi) \mid r^2 \sin^2(\theta) R_{nl}(r) Y_{lm}(\theta,\phi) \rangle = \overbrace{\int R_{nl}^2 r^4 dr}^{\text{First Factor}} \underbrace{\int Y_{lm}^*(\theta,\phi) \sin^2(\theta) Y_{lm}(\theta,\phi)\, d\Omega}_{\text{Second Factor}}, \tag{3.67}$$

where the integral over r is from 0 to infinity and $d\Omega = sin(\theta)\, d\theta d\phi$ and ϕ is integrated from 0 to 2π and θ from 0 to π.

The first factor is well known [13]

$$\int R_{nl}^2 r^4 dr = \frac{n^2 a^2}{2} \left(5n^2 + 1 - 3l(l+1)\right), \tag{3.68}$$

where a is the Bohr radius, $a = \frac{\hbar^2}{\mu |q_1 q_2|}$.

We evaluate the second integral by writing $\sin^2(\theta)$ in terms of spherical harmonics

$$\sin^2(\theta) = \frac{2}{3} - \frac{4}{3}\sqrt{\frac{\pi}{5}} Y_{20}. \tag{3.69}$$

Now the second factor becomes

$$\int Y_{lm}^* \sin^2(\theta) Y_{lm} d\Omega = \frac{2}{3} \int Y_{lm}^* Y_{lm} d\Omega - \frac{4}{3}\sqrt{\frac{\pi}{5}} \int Y_{lm}^* Y_{20} Y_{lm} d\Omega. \tag{3.70}$$

Because Y_{lm} are orthonormal eigenfunctions we know $\int Y_{lm}^* Y_{lm} d\Omega = 1$. To evaluate the integral, which is the product of three spherical harmonics, we use the following identity [14]

$$\int Y_{l_3 m_3}^* Y_{l_1 m_1} Y_{m_2 l_2} d\Omega = \sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi(2l_3+1)}} \langle l_1 l_2 00 \mid l_1 l_2 l_3 0 \rangle \langle l_1 l_2 m_1 m_2 \mid l_1 l_2 l_3 m_3 \rangle \tag{3.71}$$

where $\langle l_1 l_2 00 \mid l_1 l_2 l_3 0\rangle$ are Clebsch-Gordan coefficients. In our case we have,

$$\int Y_{lm}^* Y_{20} Y_{lm} d\Omega = \sqrt{\frac{5}{4\pi}} \langle 2l00 \mid 2ll0\rangle \langle 2l0m \mid 2llm\rangle. \tag{3.72}$$

Analytical expressions for the Clebsch-Gordan coefficients are found using computer software,

$$\langle 2l00 \mid 2ll0\rangle = -l\,(1+l)\sqrt{\frac{1+2l}{8l^5+20l^3+10l^4-5l^2-3l}}, \tag{3.73}$$

$$\langle 2l0m \mid 2llm\rangle = -\left(l+l^2-3m^2\right)\sqrt{\frac{1+2l}{8l^5+20l^3+10l^4-5l^2-3l}}. \tag{3.74}$$

With this information the second factor is

$$\int Y_{lm}^*(\theta,\phi)\sin^2(\theta)\,Y_{lm}(\theta,\phi)\,d\Omega = \frac{2\left(l^2+l-1+m^2\right)}{4l^2+4l-3}. \tag{3.75}$$

With analytic forms for both factors we have

$$\langle \psi_{nlm}(\mathbf{r}) \mid \hat{x}^2+\hat{y}^2 \mid \psi_{nlm}(\mathbf{r})\rangle = \frac{n^2a^2\left(l^2+l-1+m^2\right)\left(5n^2+1-3l^2-3l\right)}{4l^2+4l-3}. \tag{3.76}$$

Therefore

$$\langle \psi_{nlm}(\mathbf{r}) \mid \hat{A}_{\mathbf{r}}^2 \psi_{nlm}(\mathbf{r})\rangle = \frac{B_o^2}{4}\frac{n^2a^2\left(l^2+l-1+m^2\right)\left(5n^2+1-3l^2-3l\right)}{4l^2+4l-3} \tag{3.77}$$

and the first-order energy correction in terms of the quantum numbers n, l, and m is

$$E^{(1)} = \frac{n^2\left(l^2+l-1+m^2\right)\left(5n^2+1-3l^2-3l\right)}{32l^2+32l-24}\left(\frac{a^2B_o^2}{c^2}\right)\left(\frac{q_r^2}{\mu}+\frac{q_{rR}^2}{M}\right). \tag{3.78}$$

3.5 Zeeman Effect

3.5.1 Hydrogen Atom

We first consider the Zeeman effect for the hydrogen atom. The constants take on the values

$$q_1 = -e, \qquad q_2 = e = |e|$$

$$q_r = \frac{m_1 - m_2}{M} e, \qquad q_R = 0, \qquad q_{rR} = -e.$$

In this case because q_R is zero, the wave solution for $\mathbf{R}$ is that of a free particle which can have any energy, $E_R l_j(\mathbf{R}) = \frac{\hat{\mathbf{P}}^2}{2M} l_j(\mathbf{R})$. We will assume that the center-of-mass vector is stationary and therefore $E_R = 0$. We will also assume that the spin of the two particles are aligned since this is more energetically favorable. Our eigenstate energies are

$$E_{nlm} + \frac{\hbar B_o e}{2c}\left(\frac{1}{m_1} - \frac{1}{m_2}\right)\begin{bmatrix} (m+1) \\ \\ (m-1) \end{bmatrix} + E^{(1)} \tag{3.79}$$

where $E^{(1)}$ is the first-order correction for the terms that we treated as a perturbation. The energy splitting obtained agrees with that which Lamb obtained using a relativistic wave equation [2] and with what Reed and Brun obtained using a procedure similar to the one presented here [1]. Notice that in the case of positronium, $m_1 = m_2$ and we get no energy splitting which agrees with experiment [15]. For the ground state of hydrogen $n = 1$, $l = 0$, and $m = 0$

$$E^{(1)} = \frac{a^2 B_o^2}{4c^2}\left(\frac{q_r^2}{\mu} + \frac{q_{rR}^2}{M}\right) = \frac{a^2 B_o^2 e^2}{4c^2 M}\left(\frac{(m_1 - m_2)^2}{m_1 m_2} + 1\right) \tag{3.80}$$

where

$$a = \frac{\hbar^2}{\mu e^2}. \tag{3.81}$$

The two energy levels for the ground state can be written as a function of the magnetic field strength B_o

$$E_{(1)} = E_{nlm} + AB_o + CB_o^2 \tag{3.82}$$

$$E_{(1)} = E_{nlm} - AB_o + CB_o^2 \tag{3.83}$$

where

$$A = \frac{\hbar e}{2c}\left(\frac{1}{m_1} - \frac{1}{m_2}\right) \tag{3.84}$$

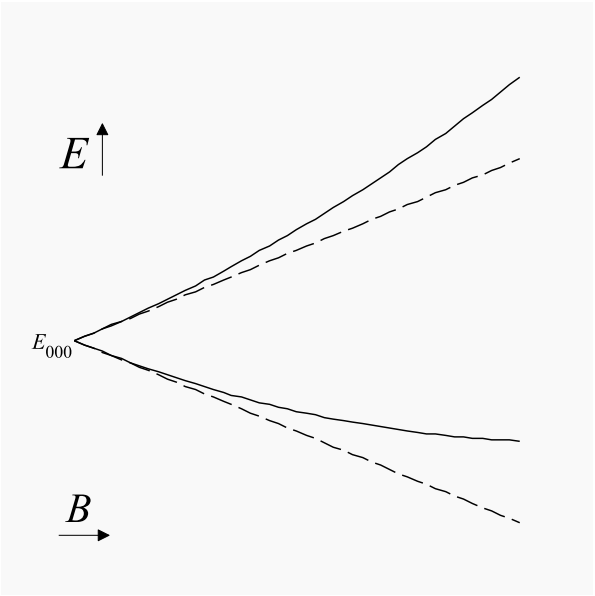

Figure 3.2 Energy versus Magnetic Field strength for the ground state energy of a hydrogen-like atom. The dotted lines represent the energy splitting obtained without the perturbation first-order energy correction and the solid lines represent the energy splitting with the first order energy correction.

and

$$C = \frac{a^2 e^2}{4c^2 M}\left(\frac{(m_1 - m_2)^2}{m_1 m_2} + 1\right). \tag{3.85}$$

The terms with B_o^2 were obtained using perturbation theory. The ratio C/A as well as magnetic field strength B_o determine the relative contribution of these perturbation terms. Fig 3.2 compares the energy splitting we obtain with and without perturbation analysis [2].

3.5.2 Helium Ion

Let us consider the Zeeman effect of a helium atom with only one electron He^+

$$q_1 = -e, \qquad q_2 = 2e$$

[2]The reader should note that without first defining m_1 and m_2 or at least C/A we cannot put any scaling on the axes of Fig 3.2.

$$q_r = e\frac{2m_1^2 - m_2^2}{M^2}, \qquad q_R = e, \qquad q_{rR} = -e\frac{m_2 + 2m_1}{M}.$$

Throughout this chapter we used a wave equation to describe two particles with spin one-half, but the nucleus of a helium atom consists of four spin one-half particles. It is expected that the protons and neutrons will pair up their spins to create a nucleus with no magnetic moment. Therefore we treat the nucleus as a particle without spin. We make this correction to Eq.(3.38) by simply removing the terms that were due to the spin of m_2. And for the energy levels we obtain the sum of the energy of a hydrogen atom not in the presence of a magnetic field, the energy associated with the center-of-mass vector, the energy of the relative-position vector in the presence in the magnetic field, and the first-order energy corrections. These energies are

$$E_{nlm} + E_{\eta_r,\eta_l,k_z} - \frac{\hbar B_o e}{2cm_1}\left(\frac{m\left(2m_1^2 - m_2^2\right)}{m_2 M} + \begin{bmatrix} 1 \\ \\ -1 \end{bmatrix}\right) + E^{(1)} \tag{3.86}$$

respectively. We now consider a helium ion in the ground state, $n = 1$, $l = 0$, $m = 0$, $\eta_r = 0$, $\eta_l = 0$. We also assume that the center-of-mass vector has no z-component of momentum and therefore $k_z = 0$ and $E_z = 0$. We find for $\eta_r = 0$, $\eta_l = 0$, and $k_z = 0$

$$E_{\eta_r,\eta_l,k_z} = \frac{\hbar B_o e}{2cM}\sqrt{\frac{\left(m_2 + 2m_1\right)^2}{m_1 m_2} + 1} \tag{3.87}$$

and the first-order energy correction is given by

$$E^{(1)} = \frac{a^2 B_o^2}{4c^2}\left(\frac{q_r^2}{\mu} + \frac{q_{rR}^2}{M}\right) \tag{3.88}$$

$$= \frac{a^2 B_o^2 e^2}{4c^2 M^3}\left(\frac{\left(m_2^2 - 2m_1^2\right)^2}{m_1 m_2} + \left(m_2 + 2m_1\right)^2\right) \tag{3.89}$$

where

$$a = \frac{\hbar^2}{2\mu e^2}. \tag{3.90}$$

Chapter 4

Matrix Factorization

4.1 Introduction

Reed and Brun present a new method using matrix factorization to produce Schrödinger-like equations that are linear and first-order in both space and time [1]. We summarize their analysis of a nonrelativistic particle of mass m confined in one dimension in a time varying potential $V(x,t)$. We then expand upon their analysis by looking at more general matrix solutions to the nonrelativistic particle. Next, we examine a single particle in an external electromagnetic field. Finally, we examine a relativistic particle in an external electromagnetic field. We examine which matrix factorizations lead to spin.

Reed and Brun first derive an expression for the momentum in time p_t in terms of the classical Hamiltonian H

$$p_t = -H = -E. \tag{4.1}$$

If the system is conservative, the last term E is constant and is the total energy of the system. However, for nonconservative systems E is not constant and does not represent the energy of the system. This accepted notation is somewhat confusing as

E often denotes energy. E as we define it is the Hamiltonian as a function of time t and p_t whereas H is the Hamiltonian as a function of the positions of all the particles in the system $(\mathbf{r}_1, \mathbf{r}_2, ...)$ and their respective momentums $(\mathbf{p}_1, \mathbf{p}_2, ...)$. It follows that for any system

$$E - H = 0. \tag{4.2}$$

If one can come up with a matrix G that contains all the terms contained in E and H, and the matrix G is singular, Reed and Brun show that through a Fourier transform one obtains a system of Schrödinger-like equations [1]. The details of this derivation are not presented here. Reed and Brun focus on matrices that are linear in the momenta $p_1, ..., p_n$ and p_t ($p_t = -E$) and matrices whose determinant is $(E - H)^l = 0$ where l is a positive integer. However the mathematical properties which Reed and Brun exploit only require that the matrix contains all the terms found in E and H, and is singular. Our investigation, for simplicity, will involve only matrices that are linear in momenta and, of course, are singular. However we do not restrict ourselves to matrices whose determinant can be written in the form $(E - H)^l = 0$.

4.2 Nonrelativistic Particle Confined to 1-D

4.2.1 The 2×2 Solution

We look for a matrix, G, that meets two conditions

i) G must be linear in momenta $p_1, ..., p_n$, and $p_t = -E$,

ii) $|G| = 0$,

where $p_1, ..., p_n$ are the generalized momentum coordinates and p_t is the generalized time momentum. For the single particle of mass m confined to one dimension in a

time varying potential $V(x,t)$, one possible matrix that meets the above conditions is

$$G = \begin{bmatrix} E - V & \frac{p}{\sqrt{2\,m}} \\ \frac{p}{\sqrt{2\,m}} & 1 \end{bmatrix}. \tag{4.3}$$

This matrix satisfies condition i) because all the elements of G are linear in p and E and condition ii) because

$$|G| = E - V - \frac{p^2}{2\,m} = E - H = 0. \tag{4.4}$$

From this matrix G one obtains Schrödinger's equation [1]. However, it is possible to generate many other matrices that satisfy conditions i) and ii). A generalized 2x2 matrix G, where $|G| = E - H = 0$ is

$$G = S^{-1} \begin{bmatrix} d\,(E - V) & \frac{f\,p}{(2\,m)^g} \\ \frac{p}{f(2\,m)^{1-g}} & d^{-1} \end{bmatrix} S \tag{4.5}$$

where S is a general transformation matrix, d, f, and g are complex constants, d and f being nonzero. To obtain a system of Schrödinger-like equations, we replace E and p with the operators $\hat{E}$ and $\hat{p}$, where

$$\hat{E} = -\frac{\hbar}{i}\,\partial_t \text{ and } \hat{p} = \frac{\hbar}{i}\,\partial_x. \tag{4.6}$$

Then we multiply the matrix G by an unknown vector ψ and set it equal to zero. (These steps are justified in [1].)

$$S^{-1} \begin{bmatrix} d\left(\hat{E} - V\right) & \frac{f\,\hat{p}}{(2\,m)^g} \\ \frac{\hat{p}}{f(2\,m)^{1-g}} & d^{-1} \end{bmatrix} S \begin{bmatrix} \psi_{\,1} \\ \psi_{\,2} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{4.7}$$

In order to compare this system of coupled differential equations to the known Schrödinger equation, we must eliminate either ψ_1 or ψ_2. To do this, we multiply

both sides of the matrix Eq.(4.7) on the left hand side by S, defining

$$S = \begin{bmatrix} s_{11} & s_{12} \\ \\ s_{21} & s_{22} \end{bmatrix} \tag{4.8}$$

and we obtain the system of two equations,

$$\left[s_{11}\, d \left(\hat{E} - V \right) + \frac{s_{21}\, f}{(2\, m)^g}\, \hat{p} \right] \psi_1 = - \left[s_{12}\, d \left(\hat{E} - V \right) + \frac{s_{22}\, f}{(2\, m)^g}\, \hat{p} \right] \psi_2 \tag{4.9}$$

$$\left[\frac{s_{21}}{d} + \frac{s_{11}}{f\ (2\, m)^{1-g}}\, \hat{p} \right] \psi_1 = - \left[\frac{s_{22}}{d} + \frac{s_{12}}{f\, (2\, m)^{1-g}}\, \hat{p} \right] \psi_2. \tag{4.10}$$

Looking at Eq.(4.10) and requiring unit consistency on both sides of the equation we obtain three possibilities for solutions, namely

1) $\frac{s_{21}}{d}\, \psi_1$ has the same units as $\frac{s_{22}}{d}\, \psi_2$, but different from other two terms,

2) $\frac{s_{21}}{d}\, \psi_1$ has the same units as $\frac{s_{12}}{f(2\, m)^{1-g}}\, \hat{p}\, \psi_2$, but different from other two terms,

3) the sum on the left side of the equation has the same units as the right without any of the individual terms having the same units.

We examine each of these three possibilities one at a time.

Possibility 1

Under this assumption Eq.(4.10) becomes two equations

$$\frac{s_{21}}{d}\, \psi_1 = -\frac{s_{22}}{d}\, \psi_2, \tag{4.11}$$

$$\frac{s_{11}}{f\, (2\, m)^{1-g}}\, \hat{p}\, \psi_1 = -\frac{s_{12}}{f\, (2\, m)^{1-g}}\, \hat{p}\, \psi_2. \tag{4.12}$$

Solving for ψ_2 in Eq.(4.11), substituting the result in Eq.(4.9) and simplifying the result yields

$$s_{11}\, s_{22} = s_{21}\, s_{12}. \tag{4.13}$$

But this means $|S| = 0$, which is impossible (a transform matrix must be nonsingular). We have obtained a contradiction and reject this possibility.

Possibility 2

Under this assumption Eq.(4.10) becomes two equations

$$\frac{s_{21}}{d}\,\psi_1 = -\frac{s_{12}}{f\,(2\,m)^{1-g}}\,\hat{p}\,\psi_2, \tag{4.14}$$

$$\frac{s_{11}}{f\,(2\,m)^{1-g}}\,\hat{p}\,\psi_1 = -\frac{s_{22}}{d}\,\psi_2. \tag{4.15}$$

Applying the operator $\hat{p}$ to both sides of Eq.(4.14), solving for $\hat{p}\,\psi_1$ and substituting the result in Eq.(4.15) yields

$$\psi_2 = \frac{s_{11}\,s_{12}}{s_{21}\,s_{22}}\,\frac{(d)^2}{(f)^2\,(2\,m)^{2-2g}}\,(\hat{p})^2\,\psi_2. \tag{4.16}$$

And similarly, solving for ψ_1 gives

$$\psi_1 = \frac{s_{11}\,s_{12}}{s_{21}\,s_{22}}\,\frac{(d)^2}{(f)^2\,(2\,m)^{2-2g}}\,(\hat{p})^2\,\psi_1. \tag{4.17}$$

The solution to an ODE in this form is

$$f\,(x) = A\,e^{kx} + B\,e^{-kx}, \tag{4.18}$$

where A and B are constants of integration and k is determined by the coefficient of the second spatial derivative in the ODE. Therefore the solutions of ψ_1 and ψ_2 can be written as

$$\psi_1 = (g_1\,(x) + g_2\,(x))\;h_1\,(t)\,, \tag{4.19}$$

$$\psi_2 = (C_3\,g_1\,(x) + C_4\,g_2\,(x))\;h_2\,(t)\,, \tag{4.20}$$

where $g_1\,(x) = C_1\,e^{kx}$, $g_2\,(x) = C_2\,e^{-kx}$, $C_{1\ldots4}$ are constants of integration, and $h_{1..2}\,(t)$ are unknown functions of time. We can now plug these solutions into Eq.(4.9), and we can separate the components of g_1 and g_2 because they are not equal for all x. Finally, we can separate the space and time derivatives because the space derivatives

are independent of time. Looking at the equations that contain time derivatives of $g_1(x)$, we obtain

$$s_{11}\, d\hat{E}\, g_1(x)\; h_1(t) = -C_3\, s_{12}\, d\hat{E}\, g_1(x)\; h_2(t)\,, \tag{4.21}$$

$$\frac{s_{21}\, f}{(2\,m)^g}\, \hat{p}\, g_1(x)\; h_1(t) = -C_3\, \frac{s_{22}\, f}{(2\,m)^g}\, \hat{p}\, g_1(x)\; h_2(t)\,. \tag{4.22}$$

To satisfy these two equations for any time t it is apparent that $h_1(t) = h_2(t)$. Also the coefficients of both equations must be equal. This leads to the contradiction that $s_{11}\, s_{22} = s_{21}\, s_{12}$ or $|S| = 0$. Therefore, we conclude that possibility 2 is impossible.

Possibility 3

Possibility 3, which happens to be the only possibility that does not yield a contradiction, is also the most difficult to solve in the general case. As stated earlier, our goal is to eliminate either ψ_1 or ψ_2; however, in this case we cannot isolate ψ_1 or ψ_2 in either Eq.(4.9) or Eq.(4.10). In Eq.(4.10) if we try solving for ψ_1 we get it in terms of ψ_2, $\hat{p}\,\psi_2$, and $\hat{p}\,\psi_1$, which yields little progress towards eliminating one of the functions. And likewise, in Eq.(4.9), we can at best solve for ψ_1 in terms of ψ_1, $\hat{p}\,\psi_1$, and $\hat{p}\,\psi_2$.

However, possibility 3 becomes easy to solve if at least one of the elements of the transform matrix S happens to be zero.

We let one element of the transform matrix S be zero. Arbitrarily we let

$$S = \begin{bmatrix} 0 & s_{12} \\ \\ s_{21} & s_{22} \end{bmatrix}. \tag{4.23}$$

We can now solve for ψ_1 in Eq.(4.10) and plug the result in Eq.(4.9), which yields the following equation for $\psi_{\ 2}$

$$\frac{\hat{p}^2}{2\,m}\, \psi_2 = \left(\hat{E} - V\right) \psi_2. \tag{4.24}$$

This is the desired Schrödinger equation. Setting other elements of S to zero also produces Schrödinger's equation. We looked at all 2×2 matrices whose determinants were $E-H$. We could not mathematically reduce all of these solutions to Schrödinger's equation. However, all matrices which could be reduced led to Schrödinger's equation. Therefore, throughout the rest of this chapter for a given size and determinant we look for only one matrix. Other matrices exist which have the same dimensions and determinant, but we do not expect them to reveal anything different about the system.

4.2.2 One 3×3 Example

A 3×3 matrix G that satisfies conditions i) and ii) is

$$\begin{bmatrix} E-V & -\frac{p}{\sqrt{2\,m}} & 0 \\ -E+V & 1 & -\frac{p}{\sqrt{2\,m}} \\ -1 & 1 & 1 \end{bmatrix}. \tag{4.25}$$

This matrix G results in the following three equations

$$\frac{\hat{p}^2}{2\,m}\,\psi_1 = \left(\hat{E}-V\right)\psi_1, \tag{4.26}$$

$$\frac{\hat{p}}{\sqrt{2\,m}}\,\psi_1 = \psi_2, \tag{4.27}$$

$$\psi_3 = \psi_1 - \psi_2. \tag{4.28}$$

Again we have obtained Schrödinger's equation, Eq.(4.26). Notice that ψ_2 and ψ_3 are completely determined by ψ_1. It appears that we gain nothing from using matrices of greater dimensions than necessary.

4.2.3 $|G| = (E - H)^2$

We can also create a matrix that satisfies $|G| = (E - H)^2$ instead of $|G| = E - H$.

$$G = \begin{bmatrix} E - V & \frac{1}{\sqrt{2m}}p & 0 & 0 \\ \frac{1}{\sqrt{2m}}p & 1 & 0 & 0 \\ 0 & 0 & E - V & \frac{1}{\sqrt{2m}}p \\ 0 & 0 & \frac{1}{\sqrt{2m}}p & 1 \end{bmatrix} \tag{4.29}$$

This leads to two independent systems of equations

$$G_1 \begin{bmatrix} \psi_{\,1} \\ \\ \psi_{\,2} \end{bmatrix} = \begin{bmatrix} 0 \\ \\ 0 \end{bmatrix} \text{ and } G_2 \begin{bmatrix} \psi_{\,3} \\ \\ \psi_{\,4} \end{bmatrix} = \begin{bmatrix} 0 \\ \\ 0 \end{bmatrix} \tag{4.30}$$

where

$$G_1 = G_2 = G = \begin{bmatrix} E - V & \frac{p}{\sqrt{2\,m}} \\ \\ \frac{p}{\sqrt{2\,m}} & 1 \end{bmatrix}, \tag{4.31}$$

and $|G_1| = |G_2| = E - H$. We obtain two copies of Schrödinger's equation, one from G_1 and one from G_2. Throughout the rest of this chapter when looking for matrices that satisfy $|G| = (E - H)^2$, we will look for matrices that cannot be reduced to two identical matrices whose determinant is $E - H$, considering that such matrices are trivial.

4.3 Classical Particle in an External Electromagnetic Field

The Hamiltonian of a single particle in an external electromagnetic field is given by Eq.(3.1)

$$H = \frac{1}{2m}\left(\mathbf{p} - \frac{q}{c}\mathbf{A}\right)^2 + V \tag{4.32}$$

where $\mathbf{p} = (p_x, p_y, p_z)$ and $\mathbf{A} = (A_x, A_y, A_z)$ are the canonical momentum and vector potentials associated with the magnetic field. A matrix G_1 that is singular and linear in momenta that describes this system is

$$G_1 = \begin{bmatrix} E - V & \frac{1}{\sqrt{2m}}\left(p_x - \frac{q}{c}A_x\right) & \frac{1}{\sqrt{2m}}\left(p_x - \frac{q}{c}A_x\right) & \frac{1}{\sqrt{2m}}\left(p_z - \frac{q}{c}A_z\right) \\ \frac{1}{\sqrt{2m}}\left(p_x - \frac{q}{c}A_x\right) & 1 & 0 & 0 \\ \frac{1}{\sqrt{2m}}\left(p_y - \frac{q}{c}A_y\right) & 0 & 1 & 0 \\ \frac{1}{\sqrt{2m}}\left(p_z - \frac{q}{c}A_z\right) & 0 & 0 & 1 \end{bmatrix} \tag{4.33}$$

$$|G_1| = E - V - \frac{1}{2m}\left[\left(p_x - \frac{q}{c}A_x\right)^2 + \left(p_y - \frac{q}{c}A_y\right)^2 + \left(p_z - \frac{q}{c}A_z\right)^2\right] = E - H \tag{4.34}$$

We find the Schrödinger-like equation by the usual method.

$$\hat{G}_1\psi = 0 \tag{4.35}$$

$$\left[\frac{1}{2m}\left(\hat{\mathbf{p}} - \frac{q}{c}\hat{\mathbf{A}}\right)^2 + V\right]\psi_1 = \hat{E}\psi_1. \tag{4.36}$$

This is the classical Schrödinger equation we would expect, neglecting spin. The equations of ψ_2, ψ_3, and ψ_4 are completely determined by ψ_1 and do not tell us anything about the system that we could not obtain from ψ_1. We can also look for a matrix where $|G_2| = (E - H)^2 = 0$, still requiring that G_2 is linear in momenta. However before continuing, we notice that the terms that appear in Eq.(4.33) are used frequently and for simplicity we introduce these new terms

$$E_k = E - q\phi \text{ and } T_j = \frac{1}{\sqrt{2m}}\left(p_j - \frac{q}{c}A_j\right), \tag{4.37}$$

where j is a dummy index used to represent x, y or z. One example of a matrix where $|G_2| = (E - H)^2 = 0$ that is nontrivial is

$$G_2 = \begin{bmatrix} E_k & 0 & T_z & Tx - iT_y \\ 0 & E_k & Tx + iT_y & -T_z \\ T_z & Tx - iT_y & 1 & 0 \\ Tx + iT_y & -T_z & 0 & 1 \end{bmatrix}. \tag{4.38}$$

This can be written concisely using the spin terms defined in Eq.(3.7), Eq.(3.8), and Eq.(3.9), where we have only one particle, $N = 1$, and the vector $\mathbf{T} = (T_x, T_y, T_z)$

$$G_2 = \begin{bmatrix} E_k I_2 & \hat{\sigma} \cdot \mathbf{T} \\ \hat{\sigma} \cdot \mathbf{T} & I_2 \end{bmatrix}. \tag{4.39}$$

Again, we find the Schrödinger-like equation by the usual method

$$\hat{G}_2 \psi = 0, \text{ where } \psi = \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix} = \begin{bmatrix} \chi_1 \\ \chi_2 \end{bmatrix}. \tag{4.40}$$

$$\left[E_k - \left(\hat{\sigma} \cdot \hat{\mathbf{T}}\right)\right] \chi_1 = 0 \text{ which is } \left[\frac{1}{2m}\left[\hat{\sigma} \cdot \left(\hat{\mathbf{p}} - \frac{q}{c}\hat{\mathbf{A}}\right)\right]^2 + q\phi\left(\hat{\mathbf{r}}, t\right)\right] \chi_1 = \hat{E}\chi_1. \tag{4.41}$$

We obtain Pauli's equation. Apparently, in order to satisfy $|G_2| = (E - H)^2$, G_2 linear in the momenta and nontrivial, we introduced spin-$\frac{1}{2}$. We might reasonably guess that by introducing spin-1 matrices in a similar matter, we would get a matrix G_3 such that $|G_3| = (E - H)^3$. This turns out to be incorrect.

$$G_3 = \begin{bmatrix} E_k I_3 & \hat{\sigma^1} \cdot \mathbf{T} \\ \hat{\sigma^1} \cdot \mathbf{T} & I_3 \end{bmatrix} \tag{4.42}$$

where $\hat{\sigma^1} = \left[\sigma_x^1, \sigma_y^1, \sigma_z^1\right]$ and

$$\sigma_x^1 = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \sigma_y^1 = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{bmatrix}, \text{ and } \sigma_z^1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}. \quad (4.43)$$

Instead of $|G_3| = (E-H)^3$, we get $|G_3| = E\,(E-H)^2 = 0$. G_3 is still singular and linear in momenta and therefore we can perform the quantum transformation and obtain the Pauli-like equation

$$\left[\frac{1}{2m}\left[\hat{\sigma^1}\cdot\left(\hat{\mathbf{p}} - \frac{q}{c}\hat{\mathbf{A}}\right)\right]^2 + q\phi\left(\hat{\mathbf{r}}, t\right)\right]\chi_1 = \hat{E}\chi_1. \quad (4.44)$$

We can also find two matrices G_{4a} and G_{4b} that use the spin matrices for spin-$\frac{3}{2}$ particles and lead to unique solutions

$$\sigma_x^{\frac{3}{2}} = \begin{bmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{bmatrix}, \quad (4.45)$$

$$\sigma_y^{\frac{3}{2}} = \begin{bmatrix} 0 & -i\sqrt{3} & 0 & 0 \\ i\sqrt{3} & 0 & -2i & 0 \\ 0 & 2i & 0 & -i\sqrt{3} \\ 0 & 0 & i\sqrt{3} & 0 \end{bmatrix}, \quad (4.46)$$

$$\sigma_z^{\frac{3}{2}} = \begin{bmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -3 \end{bmatrix}, \quad (4.47)$$

$$G_{4a} = \begin{bmatrix} E_k I_4 & \hat{\sigma^{\frac{3}{2}}}\cdot\mathbf{T} \\ \hat{\sigma^{\frac{3}{2}}}\cdot\mathbf{T} & I_4 \end{bmatrix} \quad (4.48)$$

where $|G_{4a}| = (E-H)^2 \left(E_k - 9\mathbf{T}^2\right)^2 = 0$,

$$G_{4b} = \begin{bmatrix} E_k I_4 & \frac{1}{3}\hat{\sigma^{\frac{3}{2}}} \cdot \mathbf{T} \\ \frac{1}{3}\hat{\sigma^{\frac{3}{2}}} \cdot \mathbf{T} & I_4 \end{bmatrix} \tag{4.49}$$

where $|G_{4b}| = (E-H)^2 \left(E_k - \frac{1}{9}\mathbf{T}^2\right)^2 = 0$. From this we obtain two Pauli-like spinor equations

$$\left[\frac{1}{2m}\left[\hat{\sigma^{\frac{3}{2}}} \cdot \left(\hat{\mathbf{p}} - \frac{q}{c}\hat{\mathbf{A}}\right)\right]^2 + q\phi\left(\hat{\mathbf{r}}, t\right)\right]\chi_1 = \hat{E}\chi_1, \tag{4.50}$$

$$\left[\frac{1}{18m}\left[\hat{\sigma^{\frac{3}{2}}} \cdot \left(\hat{\mathbf{p}} - \frac{q}{c}\hat{\mathbf{A}}\right)\right]^2 + q\phi\left(\hat{\mathbf{r}}, t\right)\right]\chi_1 = \hat{E}\chi_1. \tag{4.51}$$

4.4 Relativistic Particle Confined to 1-D

The Hamiltonian for a single relativistic particle of rest mass m confined to motion in one dimension in a time varying potential $V(x,t)$ is

$$H = E = \sqrt{m^2c^4 + c^2p^2} + V, \tag{4.52}$$

which is equivalent to the following expression:

$$(E - V + cp)(E - V - cp) - m^2c^4 = 0. \tag{4.53}$$

We seek a matrix G that is singular and linear in momenta. Let

$$G = \begin{bmatrix} E - V + cp & 0 & 0 & 1 \\ 0 & E - V - cp & 1 & 0 \\ m^2c^4 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix}. \tag{4.54}$$

We have $|G| = (E - V + cp)(E - V - cp) - m^2c^4 = 0$. This matrix leads to the wave equation

$$c^2\hat{p}^2\psi_1 = \left(\hat{E} - V\right)^2 \psi_1 - m^2c^4\psi_1, \tag{4.55}$$

which can be written

$$c^2\hat{p}^2\psi_1 + m^2c^4\psi_1 = \left(\hat{E} - V\right)^2 \psi_1. \tag{4.56}$$

This is the Klein-Gordon Equation.

4.5 Relativistic Particle in an External Electromagnetic Field

The Hamiltonian of a relativistic particle in an external electromagnetic field is

$$H = E = \sqrt{m^2c^4 + (c\mathbf{p} - q\mathbf{A})^2} + V. \tag{4.57}$$

We define the following new terms before defining the matrix G

$$E_k = E - V \text{ and } T_j = (cp_j - qA_j) \tag{4.58}$$

and $\mathbf{T} = (T_x, T_y, T_z)$. A matrix G that is singular in momenta and represents the Hamiltonian is

$$G = \begin{bmatrix} E_k I_2 + \hat{\sigma}\cdot\mathbf{T} & 0_2 & 0_2 & \sigma_x \\ 0_2 & E_k I_2 + [-\sigma_x, \sigma_y, \sigma_z]\cdot\mathbf{T} & \sigma_x & 0_2 \\ 0_2 & \sigma_x & 0_2 & \sigma_x \\ \sigma_x m^2c^4 & 0_2 & \sigma_x & 0_2 \end{bmatrix} \tag{4.59}$$

where 0_2 is a 2×2 matrix of zeros. Here $|G| = \left(E_k^2 - \mathbf{T}^2 - m^2c^4\right)^2 = 0$. And from this we obtain the Klein-Gordon Equation with spin

$$\left[\hat{\sigma}\cdot\left(c\hat{\mathbf{p}}^2 - q\hat{\mathbf{A}}\right)\right]^2 \chi_1 + m^2c^4\chi_1 = \left(\hat{E} - V\right)^2 \chi_1 \text{ where } \chi_1 = \begin{bmatrix} \psi_1 \\ \\ \psi_2 \end{bmatrix}. \tag{4.60}$$

An alternative matrix G that represents the Hamiltonian was first given by Dirac

$$G = \begin{bmatrix} (E_k - mc^2)\, I_2 & -\hat{\sigma} \cdot \mathbf{T} \\ -\hat{\sigma} \cdot \mathbf{T} & (E_k + mc^2)\, I_2 \end{bmatrix}. \tag{4.61}$$

Here $|G| = \left(E_k^2 - \mathbf{T}^2 - m^2c^4\right)^2 = 0$. Dirac's matrix factorization is the only matrix factorization in this chapter to predict anti-particles. It has the same determinant of Eq.(4.59) but the matrix is smaller, a 4×4 matrix, whereas Eq.(4.59) is 8×8.

4.6 Conclusions

Reed and Brun have generalized the matrix factorization methods used by Dirac in the relativistic case and later Levy-Leblond in the nonrelativistic case. We looked at all possible 2×2 matrices that represented a single particle confined to one dimension in a time varying potential. We discovered that many of these matrices led to Schrödinger's equation and others seemed unsolvable by analytical techniques. Next we looked at a classical particle in an external electromagnetic potential. When requiring that $|G| = E - H = 0$, we again obtained Schrödinger's equation. When requiring that $|G| = (E - H)^2 = 0$ and the matrix G to be nontrivial, we obtained Pauli's Equation to describe a spin-$\frac{1}{2}$ particle. We also investigated singular matrices that contained matrices for spin-1 and spin-$\frac{3}{2}$ particles leading to Eq.(4.44), Eq.(4.50), and Eq.(4.51). However these equations appear to be nonphysical. For example, if we were to assume that Eq.(4.44) represented a charged particle with spin-1, then we could expect that the three spinor components should be identical in the absence of a magnetic field, because the spin would not have anything with which to interact. However by setting $\mathbf{A} = 0$, we find that the three spinor equations contained in Eq.(4.44) are not at all identical. By a similar argument Eq.(4.50) and Eq.(4.51) also appear to be nonphysical.

We next looked at a relativistic particle confined to one dimension in a time varying potential. We found a matrix G that produced the Klein-Gordon Equation. We then looked at a relativistic particle in an electromagnetic potential. By requiring $|G| = (E - H)^2 = 0$ we obtained a matrix that produced a Klein-Gordon-like equation with spin. Finally we showed that Dirac's method involved using the smallest possible matrix G that satisfied $|G| = (E - H)^2 = 0$. Dirac's equation not only includes spin, it includes anti-particle solutions as well.

Based on the patterns found in these examples we draw the following conclusions:

1) The equations obtained from matrices that satisfy $|G| = E - H$ can be obtained without matrix factorization at all, by simply turning the classical quantities E, $\mathbf{p}$, $\mathbf{A}$, etc. into their respective quantum operators and have them operate on a wave function ψ.

2) Spin-$\frac{1}{2}$ equations for a given system, relativistic or not, are obtained by looking for matrices whose determinants are $|G| = (E - H)^2$ and that are nontrivial, or in other words cannot be separated into two matrix equations that both satisfy $|G| = E - H$. (For an example of a trivial solution see Eq.(4.30).)

3) Anti-particle solutions are obtained by the relativistic model only, and specifically are obtained by the smallest matrix G that satisfies the same condition required to introduce spin, namely $|G| = (E - H)^2$.

Chapter 5

Conclusions

In Chapter 2 we looked at two classical particles in an external homogeneous magnetic field. We first examined the necessary conditions for a system to use equations that ignore relativity, gravity, energy loss due to radiation, and quantum mechanics. We then used these equations to examine the two particle system using the center-of-mass vector and the relative-position vector. We defined three charges to help characterize the system, the total charge q_R, the reduced charge q_r, and the interactive charge q_{rR}. We then examined boundedness in the plane perpendicular to the B-field. We argued that the center-of-mass vector would be bounded in this plane unless the total charge was zero and that the relative-vector is always bounded in this plane. We used numerical simulations to confirm these results.

There are many ideas to explore that are not included in Chapter 2. The arguments for the conditions of boundedness fall short of an analytic proof and could be strengthened. Also, Chapter 2 does not investigate motion in the direction of the B-field. The center-of-mass vector has no force that acts in the direction of the B-field. However, the relative-position vector components in the plane perpendicular to the B-field are coupled to the component in the direction of B-field by the electric force

interaction between the particles. This could lead to some interesting cases where momentum of the relative-position vector in the B-field direction first gets transferred to the plane perpendicular to the B-field, and then to the center-of-mass vector. Finally, Chapter 2 never looked at including terms to account for relativity, gravity, radiation loss, or quantum mechanics. It would be interesting to examine what happens when one includes some correction terms to account for one or more of these ideas.

In Chapter 3 we used the new charges from Chapter 2 to examine two quantum particles with spin in an external homogeneous magnetic field. We examined the Zeeman effect for hydrogen, positronium, a positive helium ion, and other hydrogen-like ions. Throughout our analysis, we did not make use of the total pseudomomentum, and it is not clear if doing so would provide any advantages. We also focused on the energy levels and did little work to examine the wave functions of such systems. We did not discuss what transitions are allowed and what transitions are forbidden for Hydrogen-like atoms in a homogeneous magnetic field. However, such a discussion is found in a work by P. Schmelcher and L. S. Cederbaum [4]. Finally, it would be interesting to include an external homogeneous electric field and see what effect such an addition would have on energy levels and wave functions.

In Chapter 4 we examined the types of equations one could form using a matrix factorization technique. Using this technique we were able to derive Schrödinger wave equations, Pauli wave equations, Klein-Gordon wave equations, and Dirac wave equations. However we also derived equations that appear to be nonphysical. Based on all the different factorizations, we postulated what conditions would lead to the different equations listed above. It would be interesting to try and prove or disprove any of the postulates presented at the end of Chapter 4. It also remains an open question as to why some factorizations predict spin or antiparticles and some do not. Even though some equations appear to be nonphysical, it would interesting

to investigate how particles would act if they obeyed these equations. Perhaps the equations do represent something physical, or perhaps it would be interesting to compare and contrast their predictions to physical systems.

Appendix A

Maple© Code for Trajectories of Particles

The following Maple© code was used for the simulations described in Chapter 2. The code does not have all the simulations or graphs in Chapter 2, but instead contains the general outline to conduct simulations and graph the motion of two classical particles in a uniform magnetic field with chosen initial conditions. The code was written in Maple© Version 11. Please contact the author for the actual files used to produce the graphs in this thesis.

```
> restart:mu:=m1*m2/(m1+m2): M:=m1+m2:mu:=m1*m2/(m1+m2): M:=m1+m2:
```

We record the equations of motion.

```
> Eq7:=m1*diff(r1z(t),t$2)=+Z*q1*q2*(r1z(t)-r2z(t))/((r1x(t)-r2x
  (t))^2+(r1y(t)-r2y(t))^2+(r1z(t)-r2z(t))^2)^(3/2):
> Eq8:=m1*diff(r1x(t),t$2)=(q1)/(c)*B*diff(r1y(t),t)+Z*q1*q2*(r1x
  (t)-r2x(t))/((r1x(t)-r2x(t))^2+(r1y(t)-r2y(t))^2+(r1z(t)-r2z(t))
  ^2)^(3/2):
> Eq9:=m1*diff(r1y(t),t$2)=-(q1)/(c)*B*diff(r1x(t),t)+Z*q1*q2*(r1y
  (t)-r2y(t))/((r1x(t)-r2x(t))^2+(r1y(t)-r2y(t))^2+(r1z(t)-r2z(t))
  ^2)^(3/2):
> Eq10:=m2*diff(r2z(t),t$2)=+Z*q1*q2*(r2z(t)-r1z(t))/((r1x(t)-r2x
  (t))^2+(r1y(t)-r2y(t))^2+(r1z(t)-r2z(t))^2)^(3/2):
> Eq11:=m2*diff(r2x(t),t$2)=(q2)/(c)*B*diff(r2y(t),t)+Z*q1*q2*(r2x
  (t)-r1x(t))/((r1x(t)-r2x(t))^2+(r1y(t)-r2y(t))^2+(r1z(t)-r2z(t))
  ^2)^(3/2):
> Eq12:=m2*diff(r2y(t),t$2)=-(q2)/(c)*B*diff(r2x(t),t)+Z*q1*q2*
  (r2y(t)-r1y(t))/((r1x(t)-r2x(t))^2+(r1y(t)-r2y(t))^2+(r1z(t)-r2z
  (t))^2)^(3/2):
```

We start out with q_R being zero. We choice Z and c to work in SI units. We also record the initial conditions for similuation one.

```
> Z:=8.987551787*10^9:c:=1;m2:=2;m1:=1;q2:=1/sqrt(Z):q1:=-1/sqrt
  (Z):B:=1000:r2xo:=1.5:r2yo:=0;r2zo:=0;Dr2xo:=0:Dr2yo:=
  -.25/2:Dr2zo:=0:r1xo:=-1.5;r1yo:=0:r1zo:=0:Dr1xo:=0:Dr1yo:=
  .25:Dr1zo:=0:tt:=20:alphacsqrt:=(r1xo-r2xo)*c^2:
> IC:=rx(0)=r1xo-r2xo,ry(0)=r1yo-r2yo,rz(0)=r1zo-r2zo,D(rx)(0)=
  Dr1xo-Dr2xo,D(ry)(0)=Dr1yo-Dr2yo,D(rz)(0)=Dr1zo-Dr2zo,Rx(0)=1/M*
  (m1*r1xo+m2*r2xo),Ry(0)=1/M*(m1*r1yo+m2*r2yo),Rz(0)=1/M*(m1*
  r1zo+m2*r2zo),D(Rx)(0)=1/M*(m1*Dr1xo+m2*Dr2xo),D(Ry)(0)=1/M*(m1*
  Dr1yo+m2*Dr2yo),D(Rz)(0)=1/M*(m1*Dr1zo+m2*Dr2zo);IC2:=r1x(0)=
  r1xo,r1y(0)=r1yo,r1z(0)=r1zo,D(r1x)(0)=Dr1xo,D(r1y)(0)=Dr1yo,D
  (r1z)(0)=Dr1zo,r2x(0)=r2xo,r2y(0)=r2yo,r2z(0)=r2zo,D(r2x)(0)=
  Dr2xo,D(r2y)(0)=Dr2yo,D(r2z)(0)=Dr2zo:
```

We solve the equations and plot what we are interested in.

```
> XX2:=dsolve({Eq7,Eq8,Eq9,Eq10,Eq11,Eq12,IC2},{r1x(t),r1y(t),r1z
  (t),r2x(t),r2y(t),r2z(t)},type=numeric,maxfun=-1);with(plots)
  :odeplot(XX2,[[r1x(t),r1y(t)],[r2x(t),r2y(t)]],0..tt,numpoints=
  3000,color=[red,green]);odeplot(XX2,[[r1x(t)-r2x(t),r1y(t)-r2y
  (t)],[(1/M)*(m1*r1x(t)+m2*r2x(t)),(1/M)*(m1*r1y(t)+m2*r2y(t))]],
  0..tt,numpoints=3000,color=[red,green]);
> odeplot(XX2,[[t,sqrt(diff(r1x(t),t)^2+diff(r1y(t),t)^2)],[t,sqrt
  (diff(r2x(t),t)^2+diff(r2y(t),t)^2)]],t=0..tt,numpoints=3000,
  color=[red,green]):
```

Figure A.1 Maple© Version 11 code to simulate two charged particles in a uniform magnetic field (output suppressed).

Appendix B

Maple© Code for Energy Corrections for Two Quantum Particles

The following Maple© code was used for the energy corrections listed in Chapter 3. The code shows how the energy corrections were calculated and could be used to calculate energy corrections not listed in Chapter 3. The code was written in Maple© Version 11. Please contact the author for the actual files used to generate the energy-correction terms used in this thesis.

```
> restart:assume(a>0);
```

We First create a function psi2(n,l,m) to represent the hydrogen wave solutions this is the solution to the relative position vector r

```
> Pl:= (m,l)-> if abs(m)>0 then (-1)^m*sin(theta)^abs(m)*diff(P(l)
  ,x$abs(m))  else (-1)^m*sin(theta)^abs(m)*(P(l)) end if:
> P:=l-> if l>0 then 1/2^l*1/l!*diff((x^2-1)^l,x$l) else 1 end if:
> Y:=(m,l)->if m>-1 then sqrt((2*l+1)*(l-m)!/(l+m)!/(4*Pi))*subs
  (x=cos(theta),Pl(m,l))*exp(i*m*phi) else sqrt((2*l+1)*(l-m)!/(l+
  m)!/(4*Pi))*subs(x=cos(theta),Pl(m,l))*exp(i*m*phi)*(l-abs(m))!/
  (l+abs(m))!*(-1)^(m) end if:
> L:=(alpha,nprime)-> if nprime>0 then x^(-alpha)*exp(x)/nprime!*
  diff(exp(-x)*x^(nprime+alpha),x$nprime) else 1 end if :
> psi:=(n,l,m)->sqrt((2/(n*a))^3*(n-l-1)!/(2*n*((n+l)!)^1))*exp(-
  x/2)*x^l*L(2*l+1,n-l-1)*Y(m,l):
> psi2:=(n,l,m)->subs(x=2*r/(a*n),psi(n,l,m)):
> psi2conj:=(n,l,m)->subs(i=-i,psi2(n,l,m)):
```

We now do the same for the wave solutions of Landau Problem this is the solution for the center of mass position vector

```
> Her:=n->if n>0 then (-1)^n*exp(x^2)*diff(exp(-x^2),x$n) else 1
  end if:
> HerNew:=n->(M*w/(Pi*hbar))^(1/4)*1/sqrt(2^n*n!)*subs(x=sqrt(M*
  w/hbar)*(X-hbar*ky*c/(q_R*B_o)),simplify(Her(n))*exp(-x^2/2+i*
  ky*Y+i*kz*Z)):
> HerFinal:=n->subs(w=q_R*B_o/(c*M),HerNew(n)):
> HerFinalconj:=n->subs(i=-i,HerFinal(n)):
```

FF and FFconj are the overall wave function.

```
> FF:=(n,l,m,n2)->psi2(n,l,m)*HerFinal(n2):
> FFconj:=(n,l,m,n2)->psi2conj(n,l,m)*HerFinalconj(n2):
> xx:= r*sin(theta)*cos(phi): yy:=r*sin(theta)*sin(phi):
```

All Ar ^2 terms

```
> Arsqrtterms:=q_rR^2/c^2*1*B_o^2*(1/(2*mu)*(X^2)+1/(8*M)*(xx^2+
  yy^2))+q_r^2/c^2*1/4*B_o^2*1/(2*mu)*(xx^2+yy^2);
> expand(int(int(int(int(FFconj(aa, bb, cc, dd)*Arsqrtterms*FF(aa,
  bb, cc, dd)*r^2*sin(theta),r=0..infinity),theta=0..Pi),phi=0..2*
  Pi),X=-infinity..infinity));
> aa:=1:bb:=0:cc:=0:dd:=1:expand(int(int(int(int(FFconj(aa, bb,
  cc, dd)*Arsqrtterms*FF(aa, bb, cc, dd)*r^2*sin(theta),r=0..
  infinity),theta=0..Pi),phi=0..2*Pi),X=-infinity..infinity));
```

Figure B.1 Maple© Version 11 code used to calculate first order energy corrections (output suppressed).

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