Nonlinear dynamics of a particle in an electric and magnetic field

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Nonlinear dynamics of a particle in an electric and magnetic field

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NONLINEAR DYNAMICS OF A PARTICLE
IN AN ELECTRIC AND MAGNETIC FIELD

by

Sean Doyle

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

Master of Science

in

Physics

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University of Nevada, Las Vegas
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University of Nevada Las Vegas
August 1992
ABSTRACT

This work involves the computational study of a charged particle (electron) in the field of a heavy particle (proton) and an applied constant magnetic field. When either the magnetic field or the central field of the proton are "switched off", closed analytic solutions for the classical dynamics exist. However, when both fields are present, only approximate analytic solutions are available. For a weak, applied magnetic field perturbation theory may be used to construct the approximate solutions, but these solutions break down in the high field regime. To study the behavior of such an atom in this region we perform numerical studies of the classical dynamics. The nonlinear terms in the equations of motion induce chaotic motions, and such effects will be explored in detail.
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1 Introduction.

Poincare was the first to show that solutions to Newton's equations of motion may be unstable in simple dynamic systems[1]. For a three body system, such as models for planetary motion, Poincare showed[1] that the small perturbations induced by a less massive third body on the two planet system, may result in unpredictable trajectories. The notion that small perturbations in initial conditions lead to large deviations in trajectories, went against the prevailing view of the time. This phenomena is now called sensitive dependence of trajectories on initial conditions[2], and is one of the most recognized characteristics of chaotic systems.

The dynamics of chaotic systems can be modeled by systems of nonlinear differential equations. It is the nonlinear terms in these equations that cause large deviations in trajectories. Nonlinear equations are sometimes solved using linearized approximations, but such calculations require numerical methods whose implementation demands the use of a computer[3]. Although the computers of the 1960's were less advanced than present day computers, they allowed the numerical computations of previously time demanding analytical calculations. At this time, computer studies of dynamic
systems attracted attention to the peculiar properties of nonlinear systems. Lorenz's[3] mathematical simulations of the differential equations modeling atmospheric dynamics, again focused attention on Poincare's earlier work dealing with the instability of simple dynamic systems.

The coupled differential equations that Lorenz considered are:

\begin{align*}
(1.1) \quad \frac{dx}{dt} &= q(y - x) \\
(2.1) \quad \frac{dy}{dt} &= rx - y - xz \\
(3.1) \quad \frac{dz}{dt} &= xy - bz
\end{align*}

\( x \) is the intensity of convection motion.

\( y \) is the temperature difference between ascending and descending air.

\( z \) is the distortion of vertical temperature profile from linearity.

\( q \) is the Prantl number, used in dimensional analysis of convection in a fluid due to the presence of a hot body.
\( r \) is the normalized Rayleigh number.

\( b \) is a geometric factor.

The equations result from Rayleigh’s mathematical models of dynamic systems that behave like a fluid, such as water or a gas. Equilibrium in this model, the pure conduction state between two heating plates, where heat is transferred uniformly by the collision of the liquids molecules, is measured by the Rayleigh number. The Rayleigh number is proportional to the temperature difference between two heating plates. For a critical value of the Rayleigh number, the pure conduction state becomes unstable and perturbations in the steady flow of heat occur. This unstable state results in convection rolls\([4]\), or vortex-like dynamics in the fluid motion.

Solutions to the Rayleigh equations, that model the dynamical behavior of fluids, require a numerical expansion. Lorenz considered a simplified approximation to the Rayleigh model and studied the amplitudes for the magnitude of \( \frac{dx}{dt} \), \( \frac{dy}{dt} \), \( \frac{dz}{dt} \) in equations 1.1 through 3.1, as a function of time. Equations 1.1 through 3.1 where obtained by using this simplified approximation.

In solving Equations 1.1 through 3.1 Lorenz found that by truncating
the result of a calculation the truncation error grew during subsequent iterations. This is illustrated in the table below, note that at the end of the calculation the truncation error leads to a very large error in the final result. This behavior is one of the manifestations of sensitive dependence on initial conditions.

<table>
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<tr>
<th>evaluations</th>
<th>without interrupt</th>
<th>with interrupt</th>
</tr>
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<tr>
<td>2</td>
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<tr>
<td>10</td>
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</tr>
<tr>
<td>10</td>
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</tr>
<tr>
<td>15</td>
<td>1.2670261775</td>
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</tr>
<tr>
<td>100</td>
<td>0.7355620299</td>
<td>1.327362739</td>
</tr>
</tbody>
</table>

Chaotic dynamics, refers to the deterministic development of a systems dynamics with chaotic results[5]. In a chaotic system, the system evolves
in a deterministic pattern in which the current state of a system's dynamics depends on the previous state. In contrast, in a random system there is no connection between the present state with the previous state.

In his simplified version of the Rayleigh model of thermal convection, Lorenz discovered that in this completely deterministic system of three ordinary differential equations, all nonperiodic solutions were bounded, condition (d.) below, but unstable. They underwent irregular fluctuations without any element of randomness introduced from the outside[5]. Such fluctuations of a isolated system are the essence of chaos. All motion of a chaotic system is connected by feedback[1]. This feedback mechanism in the dynamics of the system is what leads to chaos. For example, in the weather system studied by Lorenz, the convection and conduction current interact and feed back into each other in a cyclic pattern, and results in irregular fluctuations in the dynamics of the weather.

Several conditions must be met for chaos to occur[2]:

(a.) Three independent variables.

(b.) Equations contain a nonlinear coupling term.

(c.) Divergence of trajectories.
(d.) Confinement of motion to a finite region of phase space.

(e.) Uniqueness of trajectories.

These conditions do not mean that chaos will definitely occur, and one must be careful in assuming that a system is chaotic if only some of these conditions are met.

Unpredictable behavior in chaotic systems occurs in the time evolution of a system. The phenomena manifest itself in systems ranging from the simple pendulum, to lasers, to planetary motion. The main characteristic of chaos in these systems is that they do not repeat their past behavior.

Computer simulation of the operation of lasers exhibit chaos, but many practical lasers do not operate within the parameter range where chaos occurs[2]. In these lasers a relaxation of certain physical parameters called the population inversion, $D$, a population inversion occurs when an atom is an excited state instead of the normal ground state, and the polarization, $P$, cause an effective reduction from the necessary three independent variables, to only one. This reduction of variables makes chaos impossible. The laser equations are as follows:
\[
\frac{dE}{dt} = k(-E + P)
\]
\[
\frac{dP}{dt} = Y_o(ED - P)
\]
\[
\frac{dD}{dt} = Y_1[(Y_2 + 1) - D - Y_2EP]
\]

E represents the electric field.

P represents the polarization.

D represents a population inversion.

k is the decay rate in the laser cavity due to beam transmission.

\(Y_o\) is the decay rate of the polarization.

\(Y_1\) is the decay rate of the population inversion.

\(Y_2\) is the pumping energy parameter.

Planetary chaos explains why there are gaps in the asteroid belt[1]. For example, asteroids in the asteroid belt are perturbed by the gravitational pull of Jupiter, and if two orbits of Jupiter take as long as five orbits of an asteroid, there is a 2/5 or 0.4 resonance. An asteroid caught between resonances may go into chaotic orbits or be thrown out of its orbit and escape
as a comet. These gaps in the asteroid belt are known as Kirkwood gaps[6].

Chaos in Hamiltonian systems, like the Jupiter asteroid system, is explained by the KAM theorem[6]. This theorem states that under small perturbations, a Hamiltonian system will remain stable except for small bands of instability that correspond to resonance between the original system, the asteroid and the sun in this example, and the disturbance(perturbation), the planet Jupiter. The resonance occurs when the ratio of the periods of a planet and the asteroid is a rational number like 0.333[1].

Another feature of chaos is the extreme sensitivity to the initial conditions[7]. If the system evolves from two initial conditions which differ by decimal values, the two trajectories will display a different dynamical evolution, and diverge in time. The divergence of trajectories growing exponentially in time, is described by the Lyapunov exponent, which gives the average rate of divergence[2] of the systems trajectories.

Information about chaotic systems can be obtained using phase space diagrams such as the one dimensional plot of velocity vs. displacement[8]. The simple pendulum can be used to demonstrate the use of phase space diagrams, and explain the concept of the limit cycle. The limit cycle[9] is another feature of chaotic dynamical systems, that occurs in patterns unique
Figure 1: Phase space for the undamped pendulum
to the dynamical system, as they approaches chaos.

The undamped pendulum is an example of a nondissipative energy con­served system. This system has no frictional force to restrict its motion and
has a limit cycle of a simple ellipse shown in Fig-1. Figure-1 is a one dimen­sional plot of the velocity versus the displacement. From the graph it can be
seen that the velocity $V_x$ is at its maximum value at $x=0$, and is zero when
$x$ is at its maximum value of approximately $x=1.47$. Any point in the phase
space of the undamped pendulum will settle on this elliptical limit cycle[8],
and is the cycle which the system will converge to.

Another concept required to understand chaos is the limit point. Con-
Consider the simple damped pendulum. This is a nonconservative, dissipative system losing energy due to frictional forces interfering with its motion. The limit point, shown in Figure 2, for this system is the origin of the phase space, which is the point in phase space where the damped pendulum will settle. The point of convergence of the nonconserved damped pendulum and the cycle of the undamped pendulum are called attractors. The limit point is a static, or fixed point attractor and represents static equilibrium. The limit cycle of the undamped pendulum is a periodic attractor since it has a nonstatic cyclical attractor.

A numerical analogy of a the limit point for the damped pendulum is

Figure 2: Phase space for the damped pendulum
the iteration of the function $y = \sqrt{x}$, on the interval $x \in (0,1)$. Entering any number between zero and one in this function and continually taking the square root of the result, and the square root of that result, results in a final convergence to the number one. This is an example of a limit point in an iterative numerical calculation. These concepts are used in the analysis and recognition of chaotic systems.

In section 2 the Duffing oscillator, a forced nonlinear differential equation which is known to display chaos, will be analyzed. The special case where it is possible to calculate the Lyapunov exponent by analytical methods will be examined. The Duffing oscillator models systems with a damping force, a spring force, and a cubic nonlinear term which results from the nonlinear response of the forcing term, $f$, in equation 1.2.0. The human heart has been modeled by Duffing's equations[10]. In sections 3 and 4 the concept of period doubling and the universality in chaos will be examined. These sections will show how apparently unrelated systems show clear patterns of chaotic similarity. The remainder of the work will discuss research on the computer modeling of the Lorentz equations, when applied to a hydrogen atom in an electric and magnetic field.

The experimental study of the hydrogen atoms spectrum has shown evi-
dence of chaotic behavior. The ionization of electrons from the energy states corresponding to a principle quantum number, \( n \), of approximately 60, in the classical region, reveals these chaotic orbits\(^2\). Computer modeling using the classical theory of the hydrogen atom has reproduced this phenomena and opened new possibilities for the application of chaos theory to quantum mechanics\(^{11}\).

Nonlinear nonintegrable systems (systems with a perturbation) which show a transition from regularity to chaos have been studied in much detail\(^{12}\). The computational modeling of a hydrogen atom in an electric and magnetic field with no pseudomomentum most closely parallels the research discussed here. The pseudomomentum is the momentum of the center of mass. This work has shown that by plotting the motion of the center of mass, it is easier to detect chaos than when plotting the internal motion. This work was later advanced to include the case where there is a pseudomomentum, and an additional confining potential due to a finite nuclear mass\(^{12}\). My research considers the simplest model of the hydrogen atom and plots the motion of the electron in an electric and magnetic field with the proton fixed at the center of the coordinate system.
2 The Duffing Oscillator, The Lyapunov Exponent, and Sensitivity To Initial Conditions

In analyzing the Duffing oscillator[7] we have a tool for understanding the dynamics of damped oscillation, undamped oscillation, forced undamped oscillation, and forced damped oscillation[13]. It is also very easy to show the sensitivity to the variation of the initial conditions, by examining the phase space diagrams. The Lyapunov exponent[2], a measure of the divergence of trajectories, can also be calculated from the Duffing system. The Duffing equation is

\begin{equation}
\ddot{x} = -(ax^3 + cx + b\dot{x}) + f\cos(x)
\end{equation}

With the choice of parameters \( a = 1, c = -1 \), where \( \dot{x} = \frac{dx}{dt} \) we obtain

\begin{equation}
\ddot{x} = -x^3 + x - b\dot{x} + f\cos(x)
\end{equation}

where \( f \) is the forcing amplitude, \( b \) is the damping coefficient.
The Lyapunov exponent can be used to determine if a system is sensitive to initial conditions, and therefore displays a necessary condition for chaos. If a system evolves from two slightly different initial states, \( x \), and \( x + L_0 \), where \( L_0 \) is a small change in the initial condition \( x \), the trajectories of these two states will diverge, if the Lyapunov exponent is positive, as the system evolves in time. The divergence after \( n \) iterations can be approximated as[2]

\[
L(n) = L_0 e^{un}
\]

where \( u \) is the Lyapunov Exponent.

\( L_0 \) is some small displacement.

\( L(n) \) is the difference in the function at \( x + L_0 \) and \( L_0 \).

\[
L(n) = f(x + L_0)^n - f(L_0)^n
\]

and \( n \) represents the number of iterations.

\[
u = \frac{log(df/dx)^n}{n}
\]
If $u$ is negative equation 1.21a says that the trajectories converge. If $u$ is positive, there is exponential growth and divergence of trajectories.

For special values of the parameters, analytic methods can be used to obtain the Lyapunov exponent. However, two conditions must be satisfied. The first condition demands that there is a stationary solution. When there is a stationary solution, defined so that, $dx/dt=G(x)=0$, an autonomous or time independent equation, the Jacobian matrix is also time independent, since time does not appear explicitly in the matrix elements, the eigenvalues of the matrix can be used to calculate the Lyapunov exponent. The second condition is that the forcing term, $f$, is equal to zero. If these two conditions are met the Duffing equation can be reduced to three first order differential equations. These equations are equations of the form, $Gx=ux$, where $u$ is the eigenvalue, or solution to the equation, and $G$ is the Jacobian matrix. The three first order equations can be solved to determine if the Lyapunov exponent is positive, and therefore causing exponential divergence in the time evolution of the system. The reduced equations are

\begin{equation}
\dot{x} = y = G_1(x,y,z)
\end{equation}
(1.2.3) \[ \dot{y} = x(1 - x^2) - by + f \cos(z) = G_2(x, y, z) \]

(1.2.4) \[ \dot{z} = \theta = G_3(x, y, z) \]

where,

\[ \dot{x} = dx/dt \]

\[ \dot{y} = dy/dt \]

\[ \dot{z} = dz/dt \]

and, \( G_1 \) designates the first order equation being in row one of the Jacobian matrix.

\( G_2 \) designates row two of the Jacobian,

\( G_3 \) designates row three of the Jacobian.
To calculate the Lyapunov exponent we use the definition of the Jacobian matrix, $G$,

$$G = \begin{pmatrix} \frac{dG_1}{dx} & \frac{dG_1}{dy} & \frac{dG_1}{dz} \\ \frac{dG_2}{dx} & \frac{dG_2}{dy} & \frac{dG_2}{dz} \\ \frac{dG_3}{dx} & \frac{dG_3}{dy} & \frac{dG_3}{dz} \end{pmatrix}$$

which using equations 1.2.2 through 1.2.4 in the Jacobian gives

$$\begin{pmatrix} 0 & 1 & 0 \\ 1 - 3x^2 & -b & -f \sin(z) \\ 0 & 0 & 0 \end{pmatrix}$$

In this special case when the forcing term, $f$, is equal to zero we can analytically calculate the Lyapunov exponents for the system of equations 1.2.2 through 1.2.4. The force is

$$F = x - x^3$$

This can be seen by recognizing that equation 1.2.3 is Newton's Second Law with the damping and periodic force added. Or, since equation 1.2.2 is $y = dx/dt$, equation 1.2.3 without the damping or periodic force is:

$$\ddot{x} = x(1 - x^2) = F$$
and therefore is zero at the critical points \( x=0, +1, -1 \). Ignoring the zero rows and columns we get a \( 2 \times 2 \) Jacobian. The entries of the third column vanish since the forcing term, \( f \), is zero. Solving for the eigenvalues using the determinate of \( G-uI=0 \), where \( u \) is the eigenvalue and 'I' is the identity matrix, we get for equations 1.2.2 through 1.2.4

\[
\begin{pmatrix}
0 - u & 1 \\
-2 & -b - u
\end{pmatrix}
\]

The eigenvalues are,

\[
u_1 = \frac{-b + \sqrt{b^2 - 8}}{2}
\]

\[
u_2 = \frac{-b - \sqrt{b^2 - 8}}{2}
\]

Depending on the value of the damping parameter \( b \), \( u_1 \), and \( u_2 \) can be equal to real or imaginary values. If \( b^2 - 8 \) is greater than zero then \( u_1 \) and \( u_2 \) are real. If \( b^2 - 8 \) is less than zero then \( u_1 \) and \( u_2 \) are imaginary. If \( b^2 - 8 \) is equal to zero then \( u_1 \) and \( u_2 \) are real. With these three possibilities, only the real part contributes to the Lyapunov exponent, since the imaginary part has an oscillatory term which does not contribute to the time average separation when calculating the Lyapunov exponent.
If we choose $b=0.5$ we get $u_1=u_2=-b/2=-0.25$. The imaginary part in $u_1$ and $u_2$ has been ignored since they do not contribute to the calculation of the Lyapunov exponent. We recognize that the third column (the $z$ component) of the Jacobian matrix always makes the corresponding Lyapunov exponent zero. Also, from the preceding analysis we found that $u_1=u_2=-0.25$ and this will give a negative Lyapunov exponent for both. We therefore have $(u_1, u_2, u_3) = (-, -, 0)$, which means that we have no chaos since there is no positive exponent to cause exponential divergence. Up to $b=\sqrt{8}$, $u_1$ will equal $u_2$, since anything less than $\sqrt{8}$ results in an imaginary part in $\sqrt{b^2-8}$. After $b=\sqrt{8}$, $u_2$ will get more negative than $u_1$ but they will both stay negative. We therefore see that in this special analytic case there can never be any chaos since there is no positive Lyapunov exponent.

To display the sensitivity to variation in the initial conditions for the forced undamped Duffing oscillator the parameter $b$ in equation 1.2.3 was set to zero to eliminate the damping force. The initial value of $y$ in equations 1.2.2 through 1.2.4 was then changed from $-1.0$ to $-2.0$ and the phase space examined to see if this change in initial conditions resulted in a difference in the phase space graphics. Note that the parameters in equation 1.2.3, $b$ and $f$, are the same and only the initial conditions are different.
Figure 3: Forced undamped Duffing oscillator phase space for initial $y$ equals -1.0

Figure 4: Forced undamped Duffing oscillator phase space for initial $y$ equals -2.0
Figure 5: Forced damped Duffing oscillator phase space for initial $y$ equal -1.0

In Fig-3 which has the initial $y$ value equal to $-1.0$ and Fig-4 which has the initial $y$ value equal to $-2.0$ we can see that there is clearly a difference in the phase space and suggests sensitivity to initial conditions. We have therefore displayed one of the characteristics of chaos in this system.

The forced damped Duffing equation is now examined. In this case all the parameters $b$, and $f$ are turned on and the initial conditions varied from the initial $y$ value equal to $-1.0$ in Fig-5 to the initial $y$ value equal to $-2.0$ in the Fig-6 and the phase space compared. Again, it is clear from the phase space graphics that initial condition sensitivity exists.
Figure 6: Forced damped Duffing oscillator phase space for initial $y$ equal -2.0

The Duffing oscillator is sensitive to initial conditions, but the other conditions previously discussed, must be met for the possibility of chaos to occur. Equation 1.2.0 has three independent variables $(y, \dot{y}, \dot{z})$, and condition (a.) is satisfied. Condition (b.) is satisfied by the $z^3$ term in the Duffing equation. Condition (c.) will be satisfied if the Lyapunov exponent is positive. Examination of the phase space shows sensitivity to initial conditions and condition (d) is satisfied. Condition (e.) is satisfied if you start the system from the same initial conditions, and parameters, and the same trajectories will appear in the phase space.
3 Period Doubling

The bifurcation diagram is a recurring pattern which turns up in many chaotic systems[6]. A graph of the logistic equation 1.3, which models the growth and decay of populations like insects is shown in Fig-7. In this plot of the population, $X_n$, versus the birthrate parameter, $A$, we can see a steady population of approximately 0.65 until the birthrate parameter $A$, becomes 3.0, at this point the graph splits into two paths. This split is known as period doubling, and signifies that the population is oscillating around two stable values, not one. It indicates that the insect population is breeding wildly for values $A=2.8$ to $A=3.0$. In the year following, from $A=3.0$ onward, the region is overpopulated and creates a larger death rate of insects. Therefore, the population jumps up and down between high and low levels (the two new branches on the diagram). For $A$ approximately equal to 3.42 to 3.45 there are four bifurcations, this is the period four region. Beyond $A=3.6$ the logistic map becomes chaotic.
4 Universality of Chaos

The onset of chaos reveals universal patterns in systems which appear to be unrelated. In biological systems involving the growth and death of an insect species there is the same pattern of chaos, bifurcation, as in a system such as the forced damped pendulum. The parameters in the biological system depends on food supply, the parameter $A$, and its place in the food chain. The parameters of a damped pendulum depend on the values of the force driving the pendulum, and the friction due to air resistance, or any combination of damping, and forcing parameters.

Common signs of chaos have been shown to reveal themselves in many
vastly different systems. In the graph of the logistic equation Fig-7 the bifurcation diagram is a graphical representations of an oscillating insect population. But, if we take an apparently different system like a forced damped pendulum, and we plot the natural frequency of the system versus the change in the forcing amplitude, it will also exhibit a similar bifurcation diagram. This similarity is not a coincidence.

Consider the equations below

\[(1.3) \quad X_{n+1} = AX_n (1 - X_n)\]

where,

- \(X_n\) is the population of the current year.
- \(X_{n+1}\) is the population for the year following \(X_n\).
- \(A\) is the growth and death parameter, which is related to the food supply.

Equations for various one dimensional iterative maps

where \(f(x) = y\)

\[(2.2) \quad f(x) = 1 - Ax^2\]
These equations look different and they are not expected to show clear patterns of chaotic similarity. In Figure-8 and Figure-9 we see that the graphs of Equation 2.2 and equation 3.2 are very similar to Fig-7.

These similarities were investigated by Feigenbaum and the universal Feigenbaum constants were discovered by him. Feigenbaum's constants are defined as follows[15]
In equation 5.1, $D_n$ is a measure of the distance to the nearest fixed point from the fixed point $x_n=0.5$. A fixed points is a point which never changes, or moves, under the iteration of a function. For example, if $f(x)$ is the function then $f(x_0)=x_0$ is a fixed point. Any iteration of the function $f(x)$ will give $f(x_0)=x_0$, or $f(f(x_0))=x_0$. The fixed point in this example represents where the population $X_{n+1}$ is not changing. The fixed points can be found from Figure-7 by drawing a horizontal line at $X_{n+1}$ equal to 0.5. The points where the line intersect the bifurcations are the fixed points[6].
Equations 5.1 and 6.1 are easily understood if one examines the logistics equation graph in Figure-7, and the graphs of Equations 2.2, and 3.2 in Figure-8 and Figure-9. Equation 5.1, and equation 6.1 measure the vertical ratios between the bifurcations. Equation 7.1 to measures the horizontal ratios between each point where a bifurcation occurs. For example, in equation 7.1 the values are as follows

\[ A_{n+1} = 3.448 \]
\[ A_n = 3.00 \]
\[ A_{n+2} = 3.520 \]

From Figure-7 it can be seen that these values are the bifurcation points on the diagram. These Feigenbaum constants are the same for all of these bifurcation systems. In our example, the Feigenbaum numbers are, \( a = \)
2.47, \( F = 6.222 \). These are approximations from the points taken from the graph. Feigenbaum calculated these in the limit as \( n \) approached infinity. Feigenbaum's values are, \( a = 2.502907 \), \( F = 4.66920 \). The Feigenbaum limit applies to all bifurcation systems, and they are universal constants[16].

The Lyapunov exponent is also a valuable tool to analyze the logistics map in Fig-7. By the definition of the Lyapunov exponent:

\[
(7.2) \quad u = \lim_{n \to \infty} \sum_{n=0}^{\infty} \log \left( \frac{df}{dx} \right)
\]

We can use the logistic equation,

\[
f = AX_n(1 - X_n)
\]

and take the derivative with respect to \( X_n \) giving

\[
(7.3) \quad u = \log |2 - A|
\]

Equation 7.3 results when \( y = f = X_n \). Solving for \( X_n \), the stationary point, the point where \( y = X_n \), and substituting into \( df/dX_n \) in equation 7.2, gives
\[ f = A(X_n) - A(X_n)^2 \]

With \( f = X_n \) we solve for \( X_n \) and get:

\[ X_n = \frac{A - 1}{A} \]

Since \( \frac{df}{dX_n} = A - 2AX_n \), substituting the fixed point into \( \frac{df}{dX_n} \) and then \( \frac{df}{dX_n} \) into Equation 7.2 gives Equation 7.3.

Looking at Fig-7 the graph of the logistic function, we substitute the value for \( A \), the growth parameter, in Equation 7.3 to see if \( u \), the Lyapunov exponent, is positive or negative. By definition a positive exponent means there is exponential growth and possible chaos, and a negative Lyapunov exponent leads to convergent nonchaotic results. If we substitute any value for \( A \), between 2.8 and 3.0 we get a negative value for \( u \) and therefore leads to convergence to a single period. This is clear from Fig-7 which shows only one period for these values. However, if we select any value from 3.1 to 4.0, the Lyapunov exponent is positive, and leads to additional bifurcations and chaos. The chaos occurs in the region after \( A = 3.8 \) where the bifurcations
become unclear and the population $X_{n+1}$ could be anywhere in the region for $A$ greater than 3.8.

5 Research

The motion of a charged particle in the magnetic field displays helix like motion. When a particle, such as an electron, has an initial velocity perpendicular to the magnetic field, it will follow the trajectory of a helix around and in the direction of the magnetic field. It does this with a constant velocity in the direction of the magnetic field, since there is no force in the direction of the magnetic field. This is a distinguishing feature of this system.

My research is focused on the dynamics of a charged particle in an electric and magnetic field, which are obtained by integrating the Lorentz equations numerically. The atomic unit scale is adopted since much of the previous work done on the hydrogen atom is modeled in these units. The numerical algorithm is fourth order Runge-Kutta[17] with stepsizes varying from $5.0 \times 10^{-4}$ atomic units of time, to 0.1 atomic units of time (1 a.u. = $2.4 \times 10^{-17}$ seconds). The system has two degrees of freedom, with the motion
constrained in the x-y plane. The Lorentz equations for this system are,

\[ \ddot{x} = W_0 \dot{y} + \left( \frac{q}{m} \right) E_z \]  

(1.4)

\[ \ddot{y} = -W_0 \dot{x} + \left( \frac{q}{m} \right) E_y \]  

(2.3)

\[ \ddot{z} = 0 \]  

(3.3)

where,

- \( q \) is the charge of the electron,
- \( B_z \) is magnetic field in z-direction, and
- \( m \) is mass of the electron.

\( W_0 = qB_z/m \) is the frequency of the system,

\( E_x, E_y, E_z \) are electric fields in the x, y, and z direction, and

\[ \dot{x} = \frac{dx}{dt}, \dot{y} = \frac{dy}{dt} \]

The coordinate system is chosen so that the proton of the hydrogen atom is at \((x, y) = (0, 0)\). The x, and y coordinates are in atomic units (1 a.u. length = \( 5.29 \times 10^{-9} \) cm). Fixing the protons coordinates is justified since the mass of the proton is 1860 times greater than the mass of the electron, and the center of mass motion will have a much smaller velocity than the electron.
We are therefore plotting the motion of the electron in the electric of the fixed proton and an external constant magnetic field.

Because the electric force and the force from the magnetic field in the Lorentz equation is directed inward toward the proton, there is no torque in the \( z \) direction.

The physical laws governing the hydrogen atom can also be understood in terms of the magnetic moment and the angular momentum. With the electron and proton in the \( x-y \) plane the angular momentum vector points in the direction of the magnetic field. In this system the magnetic field is pointing in the direction of the \( \hat{z} \)-direction. The magnetic moment for a positive charge points in the same direction as the angular momentum. The magnetic moment for the electron points in the direction opposite to the angular momentum vector at an angle of 180 degrees. The hydrogen atom will stay in the \( x-y \) plane since the torque, the cross product of the magnetic moment and the magnetic field, \( B_z \) is zero in the direction of the \( \hat{z} \).

In our study we increase the magnitude of the external magnetic field and examine the resulting trajectories in order to find patterns of chaos. Before this is done it is prudent to confirm that the simulation is stable with respect to propagating numerical errors. Since this is a central force
system, such as an electron rotating around a proton, there is no torque, and the change in the angular momentum is zero, which means the angular momentum is conserved. It is also a nondissipative system, and the energy of the system is conserved.

By setting $E_x$ and $E_y$ equal to zero in Equation 1.4 and 2.3 above it is possible to confirm that the particle in the magnetic field displaying the correct helix like motion predicted by the analytic solutions. This can be seen by examining the plot of the electrons trajectory in Fig-10. As the plot of the $x$, $y$ and time coordinates shows, this is clearly the correct helix motion. This can also be seen by the form of the analytic solutions. Solving Equations 1.4 and 2.3 analytically will give solutions of the form

$$x = \frac{c_1}{W_0} \sin(W_0 t) - \frac{c_2}{W_0} \cos(W_0 t)$$

$$y = \frac{c_3}{W_0} \sin(W_0 t) - \frac{c_4}{W_0} \cos(W_0 t)$$

Where $c_1, c_2, c_3, c_4$ are constants determined by the initial conditions, and $W_0$ is the frequency of the system.

these equations for the $x$ and $y$ coordinates result in the correct helix motion when plotted.
Figure 10: Helix when the $E$-field vanishes, and $B$ is nonzero

If we set the magnetic field equal to zero in Equations 1.4 and 2.3, and turn on the electric field we can also confirm that our numerical algorithm again gives the correct results predicted by the Lorentz equation. The plot of the $x$ and $y$ coordinates in Fig-11 confirms the accuracy of this numerical simulation giving the circular orbit expected for a bound orbit of negative total energy. In the simulations when both the $E$-field and the $B$-field are simultaneously equal to a non zero value, the energy was a constant value within acceptable limits for fourth order Runge-Kutta accuracy.

The energy of the system, $U$, is
Figure 11: Ellipse when the $B$ field vanishes, and $E$ is nonzero

\[ U = \frac{1}{2m} \tilde{P}^2 - \frac{e^2}{|\tilde{R}|} \]

where,

\[ \tilde{P} = m(\vec{p} - (e/c)\vec{A}) \]

\[ \tilde{A} = (1/2)[\vec{R} \times \vec{B}] \]

\[ \vec{R} = x\hat{x} + y\hat{y} \]

\[ |\vec{R}| = \sqrt{x^2 + y^2} \]

\[ \vec{V} = V_x \hat{x} + V_y \hat{y} \]
\[ \vec{B} = \vec{B}_z \hat{z} \]

- $e$ is the electron's charge.
- $m$ is the mass of the electron.
- $\vec{V}$ is the velocity vector.
- $\vec{R}$ is the radius vector.
- $|\vec{R}|$ is the magnitude of the radius vector.
- $\vec{A}$ is the vector potential.
- $c$ is the speed of light.
- $\vec{P}$ is the canonical momentum.
6 Traces of Chaos

6.1 Abbreviated symbols

The following symbols will be used throughout the rest of the paper:

\( B_z \) is the magnetic field.

\( X_i \) is the initial \( z \) coordinate.

\( Y_i \) is the initial \( y \) coordinate.

\( U \) is the total energy of the system.

\( t \) is the time.

\( a.u \) is atomic units.

\( s.z \) is the step size.

All these quantities are in atomic units.

Before investigating the possibility of chaos for a hydrogen atom in an electric and magnetic field, it is instructive to show what the results should actually look like. Fig-12 illustrates erratic trajectories which are a very close reproduction of what the chaotic dynamics, based on previous work[12], on
Figure 12: Example of Chaotic dynamics

the hydrogen atom, look like. The trajectories of the electron in this graph where reproduced by printing every 100 points of data which emulate the dynamics of the electron in an electric and magnetic field.

In examining the possibility of chaos in the dynamics of a charged particle in an electric and magnetic field, the possibility of sensitivity to small variations in the initial conditions of the system will be examined. This sensitivity to small changes in initial conditions is confirmed if the trajectories diverge in time. In Fig-16, and Fig-15 we show how the motion of the electron varies when we turn on both the electric and magnetic field. To check for sensitivity to initial conditions of the hydrogen atom in a electric and magnetic
field, the initial value of $x$ is changed from $X_i=0.9$ in Fig-16, to $X_i=0.6$ in Fig-15. The difference of 0.3 atomic units in the initial $x$ coordinate results in a clear difference in the dynamics of Fig-16 and Fig-15. The difference in the dynamics of the electron occurs very quickly over a time of only 50 atomic seconds. This means the trajectories are diverging in time, a necessary condition for sensitivity to initial conditions. This will be examined in more detail in another example. In these plots of the electrons trajectories the $x$ and $y$ coordinates, the time of 50 atomic units, the initial $y$ coordinate, and the magnetic field, $B_z=10$ atomic units, are the same. The stepsize is $5.0 \times 10^{-4}$.

An example of the divergence of the electrons trajectories with the time evolution of the systems is displayed in Fig-14 and Fig-13. A small variation of initial conditions, is satisfied by a change in the initial $y$ value $Y_i=0.42$ atomic units in Fig-13 to $Y_i=0.45$ atomic units in Fig-14. Each system is allowed to evolve for a time of 500 atomic seconds. The magnetic field is $B_z=30$ atomic units for the dynamics displayed in Fig-13, and Fig-14. The stepsize is $5.0 \times 10^{-3}$. Examining the two plots in Fig-13 and Fig-14, clearly shows the different trajectories. The only difference in the initial conditions of these two graphs, is that the initial $y$ value, $Y_i$, is changed by the small
increment of 0.03 atomic units. The difference in the trajectories of the electron in these two graphs is clear illustrating sensitivity to initial conditions. Examining the table below of the $y$ coordinate for times ranging from 0.5 atomic seconds to 100 atomic seconds clarifies that the trajectories are diverging in time. The table shows the difference in the $y$ coordinates as time is increased, starting at two different initial $y$ values, $Y_i=0.45$ atomic units and $Y_i=0.42$ atomic units. The increasing difference in the $y$ coordinate signifies sensitivity to initial conditions.
<table>
<thead>
<tr>
<th>time (seconds)</th>
<th>( Y_i=0.42 \text{a.u} )</th>
<th>( Y_i=0.45 \text{a.u} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5</td>
<td>0.84448</td>
<td>0.87461</td>
</tr>
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<td>1.0739</td>
<td>1.1103</td>
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<td>0.66873</td>
<td>0.77330</td>
</tr>
<tr>
<td>2.5</td>
<td>-0.082567</td>
<td>0.091433</td>
</tr>
<tr>
<td>6.0</td>
<td>-0.038723</td>
<td>0.124983</td>
</tr>
<tr>
<td>10</td>
<td>-0.30341</td>
<td>-0.44393</td>
</tr>
<tr>
<td>12</td>
<td>-0.0045439</td>
<td>0.1648018</td>
</tr>
<tr>
<td>15</td>
<td>-0.14345</td>
<td>0.11165</td>
</tr>
<tr>
<td>20</td>
<td>-1.0410</td>
<td>-1.1907</td>
</tr>
<tr>
<td>25</td>
<td>0.17056</td>
<td>0.07864</td>
</tr>
<tr>
<td>36</td>
<td>-0.0861228</td>
<td>1.011595</td>
</tr>
<tr>
<td>100</td>
<td>-0.28949</td>
<td>0.55525</td>
</tr>
</tbody>
</table>

It is instructive to use a positively charged particle in an electric and magnetic field as a counter example. This clarifies the influence of the electric force and the magnetic force on the dynamics of the hydrogen atom in an electric and magnetic field. In Fig-17 we plot the trajectories of a positive
Figure 13: $Y_i=0.42a.u, X_i=0.9a.u, U=-0.5068a.u, t=500$ sec

Figure 14: $Y_i=0.45a.u, X_i=0.9a.u, U=-0.4938a.u, t=500$ sec $dy=0.03a.u$
Figure 15: $Y_i=0.45\text{a.u}, X_i=0.6\text{a.u}, t=50\text{sec}, U=-0.4938\text{a.u}, B_z=10\text{a.u}$

Figure 16: $Y_i=0.45\text{a.u}, X_i=0.9\text{a.u}, \text{time}=50\text{sec}, U=-0.8333\text{a.u}, B_z=10\text{a.u}$
charge in an electric and magnetic field. The positively charged particle in Fig-17 rotates in a clockwise direction. This is because the initial $y$ velocity, $V_y$, in this simulation is directed in the positive $y$ direction in quadrant one of the $x$-$y$ plane at $X_x=0$, and the magnetic field, $B_z$, is directed in the time, or $z$ axis direction out of the $x$-$y$ plane. For these initial conditions the magnetic field initially pushes the positive charge in the positive $\hat{x}$ direction. As the positive charge gets farther from the proton the repulsive Coulomb force becomes weaker than the magnetic force, and the positive charge is pushed in the negative $\hat{x}$ direction by the magnetic force toward the proton in a clockwise orbit. The electric force between the positive charge and the proton is repulsive and directed away from the nucleus. When the radius gets very small, and the positive particle gets close to the proton, the Coulomb force becomes much larger than the magnetic force and pushes the positive charge away from the nucleus. The magnetic force at this point is also pointing away from the proton and also pushes the particle out and in another loop. The pattern repeats itself and generates the trajectories in Fig-17. The particle does not orbit in an ellipse around the proton, because the combined effect of the electric and magnetic force pushing it away from the proton.

The dynamics of the electron in an electric and magnetic field are different
Figure 17: $q=+q, B_z=10\, a.u., X_i=0.6\, a.u., Y_i=0.45\, a.u.$

Figure 18: $q=-q, B_z=10\, a.u., X_i=0.6\, a.u., Y_i=0.45\, a.u., t=150\, a.u.$
from that of the positive charge because the electric and magnetic force are both directed toward the proton. The electric force is attractive and directed toward the proton. The magnetic force is opposite to the magnetic force for a positive charge, and therefore directed inward toward the proton. The combined effect on the trajectories of the electron are counterclockwise elliptical orbits around the proton. The electrons dynamics are displayed in Fig-18. The torus shape of the dynamics is because the magnetic force pushes the electron in a circular orbit while the electron orbits the proton.

The trajectories plotted in Fig-15, and Fig-16 are for the electron under the influence of two central forces, the electric and magnetic force. These forces are directed toward the proton. The trajectories of the electron in Fig-15 eventually evolve into the shape of a torus like Fig-13 and Fig-14. In Fig-15 the trajectories are calculated up to a time of 50 atomic seconds. The electron in Fig-15 is rotating in a counterclockwise direction because the magnetic force pushes the electron in the negative $x$ direction toward the proton. The electron is also orbiting the proton in elliptical orbits while the magnetic force is pushing it counterclockwise in circular paths. It appears that the trajectories of the electron are favoring quadrant two and three in Fig-15. These trajectories are only modeled for 50 atomic seconds, and they
pass through the larger values of the positive $x$ coordinates if the time is increased to approximately 100 atomic seconds. The trajectories then trace out the shape of a torus. It is interesting to note that Fig-16, which is only different from Fig-15 by the change in the initial $x$ coordinate of 0.3 atomic units, has a different time evolution of the trajectories. In Fig-16, at a time of 50 atomic seconds, there is a large inner elliptical orbit around the proton, or the electron does not orbit as closely to the proton as in Fig-15. In Fig-16 the initial $x$ coordinate is $X_i=0.9$ atomic units. In Fig-15 the initial $x$ coordinate is $X_i=0.6$ atomic units. The starting coordinate closer to the proton in Fig-15 maintains trajectories with close orbits around the proton.

The system of the hydrogen atom in an electric and magnetic field should have constant energy, therefore only certain ranges of the coordinate system are applicable to this research, due to numerical instabilities. The search for numerical instabilities in certain ranges of the initial conditions for the magnetic field, the initial $x$ and $y$ coordinates, and the time, where investigated for stepsizes from $5.0 \times 10^{-4}$ to $5.0 \times 10^{-2}$.

In the dynamics of the electron in an electric and magnetic field, for an initial $x$ coordinate less than $X_i=0.9$ atomic units, for a time of 500 atomic seconds, with a stepsize of $5.0 \times 10^{-2}$, there are numerical instabilities in the
Runge-Kutta algorithm. At these initial $x$ values the energy is not constant. The magnetic field in this case is $B_z=10$ atomic units, and the initial $y$ coordinate is $Y_i=0.45$ atomic units. The search for numerical instabilities for initial conditions less than $X_i=0.9$ atomic units was done in decrements of 0.05 atomic units. In this range for $X_i$ less than 0.9 atomic units, with a stepsize of $5.0 \times 10^{-2}$ there was no sensitivity to initial conditions.

For the same initial conditions, $Y_i=0.45$ atomic units, $B_z=10$ atomic units, and a time of 500 atomic seconds, with a stepsize of $5.0 \times 10^{-2}$ the dynamics of the hydrogen atom was found to be stable for a limited range of initial $x$ coordinates greater than $X_i=0.9$ atomic units. Up to the value of $X_i=1.94$ atomic units the energy was found to be constant. At the initial $x$ value of $X_i=1.95$ atomic units the energy becomes positive, although the trajectories are closed bound orbits. This is obviously due to a numerical instability in the Runge-Kutta algorithm. The dynamics of the electron at $X_i=1.94$ atomic units and $X_i=1.95$ atomic units are exactly the same, displaying that the orbits for both initial $x$ coordinates are bound. The closed orbits for $X_i=1.95$ atomic units are displayed in Fig-19, and since they are closed orbits the positive energy must must be a numerical instability. The search of this $x$ range was done in increments of 0.01 atomic units from
$X_i = 0.9$ atomic units to $X_i = 1.95$ atomic units. There was no sensitivity to initial conditions in the range of this search.

For variations in the initial $y$ coordinate, $Y_i$, with the initial $x$ coordinate kept at $X_i = 0.9$ atomic units, and the time of 500 atomic units, the initial $y$ coordinate, $Y_i$, was searched for numerical instabilities. This search was also carried out for the motion of the electron in a electric and magnetic field.

With the initial $y$ coordinates less than $Y_i = 0.45$ atomic units, and the stepsize of $5.0 \times 10^{-2}$, with the magnetic field of $B_z = 10$ atomic units, a search for an instability in the energy was performed. The search was done in decrements in the initial $y$ coordinate of 0.01 atomic units. From $Y_i = 0.45$ atomic units to $Y_i = 0.40$ atomic units the energy remained constant to two decimal places. At $Y_i = 0.39$ atomic units the energy becomes unstable. In this range of constant energy there was no chaos or sensitivity to initial conditions.

A search for numerical instabilities with the same initial conditions and stepsize for $Y_i$ greater than 0.45 atomic units was also performed. The search started at $Y_i = 0.46$ atomic units and was continued in increments of 0.01 atomic units. The energy remained constant and negative to two decimal places until $Y_i = 0.7$ atomic units where the energy becomes unstable. The
trajectories with initial conditions from $Y_i=0.46$ atomic units to $Y_i=0.70$ atomic units formed an identical torus for all these initial points. There was no sensitivity to initial conditions in this region of investigation.

Different initial conditions for the magnetic field were also investigated for numerical instabilities. With the initial conditions $X_i=0.9$ atomic units, the time equal to 500 atomic units, and $Y_i=0.45$ atomic units, a region of numerical instability was found. For the magnetic field $B_z=10$ atomic units the energy $U=-0.494$ atomic units is constant to three decimal places. For a magnetic field of $B_z=15$ atomic units the energy $U=-0.49$ atomic units is only constant to two decimal places. At $B_z=20$ atomic units for these initial conditions the energy is not constant. For these initial conditions within the constant energy range there is no evidence for sensitivity to initial conditions in the dynamics of the electron in the electric and magnetic field. The stepsize is still $5.0 \times 10^{-2}$.

The numerical stability for different values of time was also investigated for the initial conditions $X_i=0.9$ atomic units, $Y_i=0.45$ atomic units, $B_z=10$ atomic units, and a stepsize of $5.0 \times 10^{-2}$. The time search for time less than 500 atomic units was done in decrements of $t=100$ atomic units, from $t=500$ atomic units to $t=100$ atomic units, and in decrements of $t=10$ atomic units
from $t=100$ atomic units to $t=10$ atomic units. From $t=10$ atomic units to $t=6$ atomic units the decrements were in $t=1$ atomic unit. The energy for $t=500$ atomic units was $U=-0.49$ atomic units and constant to only two decimal places. From $t=500$ atomic units to $t=300$ atomic units the energy is constant to two decimal places. From $t=300$ atomic units to $t=90$ atomic units the energy is constant to four decimal places. From $t=80$ atomic units to $t=6$ atomic units the energy is again constant to two decimal places. Since chaos occurs in the time evolution of the dynamics of the system it is necessary to use the largest time in which there are no numerical instabilities.

The time $t=500$ atomic seconds is the largest value of time with no numerical
instabilities. From the time of $t=400$ atomic seconds to the time $t=90$ atomic seconds there is no chaos, since dynamics like Fig-12 were not reproduced, and no sensitivity to initial conditions in this interval. Also, from $t=80$ atomic units to $t=6$ atomic units there was no sensitivity to initial conditions. At $t=500$ atomic units there is no chaos and no sensitivity to initial conditions. For the time greater than $t=500$ atomic units the energy was only constant for one increment of the time $t=100$ atomic units to $t=600$ atomic units. At the time $t=700$ atomic units the energy became unstable, and was not constant.

The search for numerical instabilities with a smaller stepsize of $5.0 \times 10^{-3}$ was done for the changes in the initial $z$ conditions with the magnetic field of $B_z=30$ atomic units, the initial $y$ coordinate $Y_i=0.45$ atomic units, and a time of 500 atomic units. This search was done for the initial $x$ coordinate $X_i$, less than $X_i=0.9$ atomic units, and greater than $X_i=0.9$ atomic units. The search for numerical instabilities was also done for an initial $y$ coordinate less than and greater than $Y_i$ equal to $Y_i=0.45$ atomic units. For the $Y_i$ search the initial $X_i$ value was kept at $X_i=0.9$ atomic units, with a magnetic field of $B_z=30$ atomic units.

The variation in the initial $x$ coordinate was done in steps of 0.1 atomic
units, with the magnetic field at \( B_z = 30 \) atomic units, the time at \( t = 500 \) atomic units, and the \( y \) coordinate held fixed at \( Y_i = 0.45 \) atomic units. The stepsize is \( 5.0 \times 10^{-3} \). With the initial \( x \) coordinate at \( X_i = 0.8 \) atomic units the energy \( U = -0.58947 \) atomic units, is constant to five decimal places. A decrease for \( x \) to \( X_i = 0.7 \) atomic units results in a constant energy of \( U = -0.701 \) atomic units, which is constant to three decimal places. At the initial \( x \) coordinate \( X_i = 0.5 \) atomic units the energy is not constant and cannot be used in the analysis of the electrons dynamics. The variation of the initial \( x \) coordinate shows definite sensitivity to initial conditions. A clear example of this sensitivity is the difference in the dynamics for the initial \( x \) value of \( X_i = 0.7 \) atomic units and \( X_i = 0.8 \) atomic units. The trajectories in Fig-20 for \( X_i = 0.8 \) atomic units, and the trajectories for the electron in Fig-21 for the \( X_i = 0.7 \) atomic units clearly show how the variation of 0.1 atomic units changes the dynamics of the electron in the electric and magnetic field.

The search for numerical instabilities in the initial \( x \) coordinate for values greater than \( X_i = 0.9 \) atomic units for the initial conditions \( B_z = 30 \) atomic units, \( Y_i = 0.45 \) atomic units, \( t = 500 \) atomic units, and the stepsize of \( 5.0 \times 10^{-3} \) was also done in increments of 0.1 atomic units, from \( X_i = 1.0 \) atomic units to \( X_i = 2.0 \) atomic units. At the initial \( x \) coordinate \( X_i = 2.0 \) atomic units
Figure 20: $B_z=30\text{a.u.}, X_i$ less than 0.9\text{a.u.}, for $X_i=0.8\text{a.u.}$

Figure 21: $B_z=30\text{a.u.}, X_i$ less than 0.9\text{a.u.} for $X_i=0.7\text{a.u.}$
Figure 22: \( X_i \) greater than 0.9 a.u., for \( X_i = 1.1 \), \( U = -0.341406 \text{a.u.} \)

there is a numerical instability and the energy becomes positive for bound orbits. There is definite sensitivity to a change in the initial conditions for all the increments of \( X_i = 0.1 \text{ atomic units} \) for a stepsize of \( 5.0 \times 10^{-3} \). At \( X_i = 1.1 \text{ atomic units} \) and \( X_i = 1.2 \text{ atomic units} \) there is a clear example of the sensitivity to initial conditions. In Fig-22 for the initial \( z \) value of \( X_i = 1.1 \text{ atomic units} \), and Fig-23 for the initial \( z \) coordinate of \( X_i = 1.2 \text{ atomic units} \), the sensitivity of the dynamics to the small change in initial coordinates is clear.

The search for numerical instabilities for changes in initial \( y \) coordinates for a stepsize of \( 5.0 \times 10^{-3} \), a magnetic field \( B_z = 30 \text{ atomic units} \), an initial
Figure 23: $X_i$ greater 0.9 a.u., for $X_i$=1.2 a.u, $U$=-0.2802742 a.u

$x$ coordinate $X_i$=0.9 atomic units, and a time of $t$=500 atomic seconds, was carried out for $Y_i$ less than 0.45 atomic units, and for $Y_i$ greater than 0.45 atomic units. The search was done in increments and decrements of 0.01 atomic units.

For the initial conditions described above for the initial $y$ coordinate less than $Y_i$=0.45 atomic units, the value of $Y_i$ was varied from $Y_i$=0.45 atomic units to $Y_i$=0.01 atomic units. The stepsize is $5.0 \times 10^{-3}$. Sensitivity to initial conditions is present in these changes of 0.01 atomic units in the initial $y$ coordinates for $Y_i$ less than $Y_i$=0.45 atomic units. In Fig-24 the initial $y$ coordinate is $Y_i$=0.41 atomic units, and the energy is $U$=-0.511133
atomic units, constant to six decimal places. If this is compared to Fig-13 where $Y_i=0.42$ atomic units, and the energy is $U=-0.5068$ atomic units the sensitivity to this small change of 0.01 atomic units is obvious.

With the magnetic magnetic field set at $B_z=30$ atomic units, the initial $x$ coordinate $X_i=0.9$ atomic units and a time of $t=500$ atomic seconds, the initial $y$ coordinate for $Y_i$ greater than 0.45 atomic units was varied in steps of 0.01 atomic units. The stepsize in this search is $5.0 \times 10^{-3}$. The energy for the increments of the initial $y$ coordinate was constant up to $Y_i=1.1$ atomic units. At $Y_i=1.1$ atomic units the energy $U=-0.20$ atomic units was constant to two decimal places. At $Y_i=1.2$ atomic units the energy is not constant and
Figure 25: \( y_i = 0.05 \text{a.u.}, U = -0.6094 \text{a.u.} \)

Figure 26: \( y_i = 0.001 \text{a.u.}, U = -0.61104 \text{a.u.} \)
this is the allowed \textit{y} limit in the search for chaos. In all the increments up to \( Y_i = 1.1 \) atomic units there is sensitivity to a change in the initial \( y \) coordinate. An example of the sensitivity to a change in the initial \( y \) coordinates is Fig-28, where \( Y_i = 1.0 \) atomic units, and Fig-27 where \( Y_i = 0.9 \) atomic units. The energy for Fig-27 is \( U = -0.2856 \) atomic units, constant to four decimal places, and Fig-28 is \( U = -0.243 \) atomic units, constant to three decimal places. The 0.1 atomic unit difference clearly shows sensitivity to initial conditions.

It is interesting to observe how different initial conditions can lead to the electrons trajectories avoiding a region or crossing a region in the \( x-y \) plane. An example of this is the trajectories of Fig-26 and Fig-25. Fig-26 has an initial \( y \) coordinate \( Y_i = 0.001 \) atomic units, with an energy of \( U = -0.61104 \) atomic units, constant to five places. Fig-25 has an initial \( y \) coordinate of \( Y_i \) equal to 0.05 atomic units, with an energy of \( U = -0.6094 \) atomic units, constant to four decimal places. Clearly Fig-25 has sections of darkly lined orbits, which signify that the electrons trajectories crossed that path many times. In Fig-26 there are white sections which signify that the electron did not go through those regions as often as Fig-25. The change of 0.049 atomic units resulted in this opposing effect. Also, Fig-26 has clear white regions where the trajectories of the electron do not enter.
Figure 27: $Y_i=0.9\,a.u., B=30\,a.u., U=-0.2856\,a.u$

Figure 28: $B_z=30\,a.u., Y_i=1.0\,a.u., U=-0.243\,a.u$
For the initial conditions $X_i=0.9$ atomic units, $Y_i=0.45$ atomic units, a stepsize of $5.0 \times 10^{-3}$, and a time of 500 atomic seconds, the variation of the magnetic field for values less than $B_z=30$ atomic units and greater than $B_z=30$ atomic units show sensitivity to initial conditions. The magnetic field is increased and decreased in steps of ten atomic units. The energy for these set initial conditions, and the variation in the magnetic field is always constant at $U=-0.49380$ atomic units. An example of the sensitivity to the changes in the magnetic field for the magnetic field less than 30 atomic units is the difference in the dynamics in Fig-29, for $B_z=1$ atomic unit, and an energy of $U=-0.4938$ atomic units and for the magnetic field $B_z=10$ atomic units in Fig-30. The energy is also $U=-0.4938$ atomic units for Fig-30. For the magnetic field greater than $B_z=30$ atomic units the sensitivity to initial conditions is displayed by the comparison of Fig-31 for the magnetic field $B_z=50$ atomic units, with the energy of $U=-0.49380$ atomic units, and Fig-32 for a magnetic field of $B_z=40$ atomic units. In all the variations of the magnetic field the energy stays the same, but the change in the magnetic field results in different dynamics for the electron in the magnetic and electric field.

The waveform, a plot of $x$ versus time, for the electron in a magnetic field of $B_z=30$ atomic units with initial conditions $Y_i=0.45$ atomic units $X_i=0.9$
Figure 29: $B=1.0\text{a.u.}, U=-0.4938\text{a.u}$

Figure 30: $B=10\text{a.u.}$, both energies are $U=-0.4938\text{a.u}$
Figure 31: $B_z=50\,a.u, U=-0.4938\,a.u$

Figure 32: $B_z=40\,a.u, U=-0.4938\,a.u$
atomic units and $Y_i=0.42$ atomic units, $X_i=0.9$ atomic units from Fig-13 and Fig-14 are displayed in Fig-33 and Fig-34 respectively. Although the dynamics of Fig-13 and Fig-14 are noticeably different the waveforms are very difficult to tell apart. The waveforms clearly indicate a periodic orbit in both the trajectories.

All of these dynamical models, which vary the initial conditions by small values to find patterns of chaos, result in trajectories which are periodic. The motion of the electron in the $x$-$y$ plane, with the evolution of the dynamics of the electron up the $z$-axis therefore is showing only periodic behavior. Chaos in this system would show nonperiodic trajectories. In the previous
work on the hydrogen atom in an electric and magnetic field [12] it was found that it was difficult to detect chaos by plotting the internal motion of the electron. To find chaos it was necessary to plot the center of mass motion, and to modify the numerical Runge-Kutta algorithm. In that work [12] the potential due to the finite nuclear mass was also included in the Hamiltonian equations. The system modeled in this work does not use this additional potential term in the Lorentz equations, and only models the classical motion of the electron in the electric and magnetic field. This may be reason that chaos is not occurring in this system. Since the divergence of trajectories depends on the time evolution of the system, which increases the number of
iterations, the numerical instability in the Runge-Kutta algorithm, in limiting the time span to $t=500$ atomic seconds, may also make chaos impossible.

In this examination of the motion of the electron in a electric and magnetic field, some of the necessary conditions for chaos have been satisfied. The Lorentz equations for this system do have three independent variables ($y_1$, $\dot{y}_1, y_2$)(below) as previously discussed in the necessary conditions for chaos(pages 5-6). There are actually four independent variables in this system of first order equations $y_1$, $\dot{y}_1$, $y_2$, $\dot{y}_2$, equations (i) through (iv) below. The four equations give two degrees of freedom, which is sufficient for chaos[5]. There is a nonlinear coupling term in the electric force $\frac{1.0}{(x^2+y^2)^{1/2}}$ term. The divergence of trajectories was shown in the table on page-42. The confinement of the motion to a finite region of space is clearly satisfied since the trajectories are bound orbits. The uniqueness of trajectories is also established since the dynamics starting from each variation of initial conditions can be reproduced. Finally, the most important condition for chaos, sensitivity to initial conditions, has been clearly demonstrated in the plots of the electrons trajectories. Therefore, except for condition(c.) all the conditions for chaos have been satisfied in conditions (a) through (e) on pages 5-6.
(Reduced first order Lorentz equations.)

(i) \[ y_1 = \dot{x} \]

(ii) \[ y_2 = \dot{y} \]

(iii) \[ \dot{y}_1 = W_0(y_2) + \frac{q}{m}(E_x) \]

(iv) \[ \dot{y}_2 = -W_0(y_1) + \frac{q}{m}(E_y) \]
APPENDIX 1

SYMBOLS AND UNITS USED IN THESIS:

$B_z$ is the magnetic field.

$E$ is the electric field.

$u$ is Lyapunov exponent.

$W_0$ is the frequency.

$L_n$ is the divergence of trajectories.

$G$ is the Jacobian matrix.

$a$ is the Feigenbaum number (vertical ratio).

$F$ is the Feigenbaum number (horizontal ratio).

$U$ is the energy.

$X_i$ is the initial $x$ coordinate.

$Y_i$ is the initial $y$ coordinate.
$t$ is the time.

$a.u$ is the atomic units.

$s.z$ is the step size.

$V_x$ is the velocity in $x$ direction.

1 atomic unit of time $2.4 \times 10^{-17}$ seconds.

1 atomic unit length is $5.29 \times 10^{-9}$ centimeters.

1 atomic unit energy is $4.35 \times 10^{-11}$ erg.
APPENDIX 2

PROGRAM USED IN RESEARCH.

This program uses the fourth order Runge-Kutta method to solve the Lorentz equations for a charged particle in an electric and magnetic field.
*driver for rkdumb

this is xv17.f

The check program for xv17.f is csavhe.f but wo(frequency)

must be adjusted to match the (xv17.f) frequency.

dimension vstart(4)

common /pach/x(100001),y(4,100001)

implicit double precision (a-h,o-z)

external derivs

x=0.0

x1 is the initial time.
	note that all x-variables are for time.also xt,xh,x+h in rk4.

vstart(1)=0.45

vstart(2)=0.9

vstart(3)=1.0

vstart(4)=0.0

vstart(4) is vx

vstart(3) is vy

vstart(1) is y(t)

vstart(2) is x(t)

x2=500.0

x2 is the final time

call rkdumb(vstart,vvar,x1,x2,nstep,derivs)

DO 10 i=1,nstep

k=k+1

u=1.0

q=1.0

oxo=0.3

oyo=1.0

sv=sqrt((y(3,i)**2+y(4,i)**2))

r=r-sqrt(y(1,i)**2+y(2,i)**2)

vt=sqrt((y(4,i)**2+y(3,i)**2))

w=v/vt

theta=ATAN(y(3,i)/y(4,i))

x=0.03138*y(1,i)**2*y(2,i)**2)*(b)**2

b=10.0

v=(1.0/2.0)*y(4,i)**2+0.0+y(3,i)**2.01-(1.0/z)

if (k.eq.100) then

write(6,*),x(1),y(2,i),y(1,i)

endif

if(i.eq.2000) then

write(6,*),x(1),y(2,i),y(1,i)

endif

if (l.eq.1050) then

write(6,*),x(1),y(2,i),y(1,i)

endif

if(i.eq.20000) then

write(6,*),x(1),y(2,i),y(1,i)

endif

if(i.eq.100) then

write(6,*),x(1),y(2,i),y(1,i)

endif

if(i.eq.8400) then

write(6,*),x(1),y(2,i),y(1,i)

endif

if(i.eq.8600) then

write(6,*),x(1),y(2,i),y(1,i)

endif

if(i.eq.8800) then

write(6,*),x(1),y(2,i),y(1,i)

endif

if(i.eq.8000) then

write(6,*),x(1),y(2,i),y(1,i)

endif

if(i.eq.10000) then

write(6,*),x(1),y(2,i),y(1,i)

endif

if(i.eq.100000) then

write(6,*),x(1),y(2,i),y(1,i)

endif
77 |c endf
78 |c write(6,*) t
79 |c write(6,*) y(4,1), y(2,1)
80 |c write(6,*) y(3,1), y(1,1)
81 |c if(1, q, 600000) then
82 |c write(6,*) w, theta
83 |c endif
84 |0 continue
85 |1 stop
86 |2 end
87 |3 SUBROUTINE REDUMB(VSTART,NVAR,X1,X2,NSTEP,DERIVS)
88 |4 PARAMETER (NMAX=4)
89 |5 COMMON /PATH/ XX(100001), Y(14, 100001)
90 |6 implicit double precision (a-h,o-z)
91 |7 external deriva
92 |8 DIMENSION VSTART(NVAR), Y(NMAX), DV(NMAX)
93 |9 DO 11 i=1, NVAR, 1
94 |10 Y(i)=VSTART(i)
95 |11 continue
96 |12 DO 10 K=1, NVAR, 1
97 |13 continue
98 |14 continue
99 |15 continue
100 |6 END
101 |7 SUBROUTINE RK4(V,DYDX,H,X,B,TOUT,DERIVS)
102 |8 PARAMETER (NMAX=4)
103 |9 DIMENSION Y(N), DYDX(N), YOUT(N), YT(NMAX), DYT(NMAX)
104 |10 implicit double precision (a-h,o-z)
105 |11 HH=H/6.
106 |12 XX=hh
107 |13 DO 11 i=1,N, 1
108 |14 YT(i)=Y(i)+HH*DYDX(i)
109 |15 continue
110 |16 CALL DERIVS(KH,YT,DY)
111 |17 DO 12 i=1,N, 1
112 |18 YT(i)=YT(i)+HH*DY(i)
113 |19 continue
114 |20 CALL DERIVS(KH,YT,DY)
115 |21 DO 13 i=1,N, 1
116 |22 YT(i)=YT(i)+HH*DY(i)
117 |23 continue
118 |24 CALL DERIVS(KH,YT,DY)
119 |25 DO 14 i=1,N, 1
120 |26 YT(i)=YT(i)+HH*DY(i)
121 |27 continue
122 |28 CALL DERIVS(KH,YT,DY)
123 |29 DO 15 i=1,N, 1
124 |30 YT(i)=YT(i)+HH*DY(i)
125 |31 continue
126 |32 CALL DERIVS(KH,YT,DY)
127 |33 DO 16 i=1,N, 1
128 |34 YT(i)=YT(i)+HH*DY(i)
129 |35 continue
130 |36 CALL DERIVS(KH,YT,DY)
131 |37 DO 17 i=1,N, 1
132 |38 YT(i)=YT(i)+HH*DY(i)
133 |39 YOUT(i)=YT(i)+66*(DYDX(i)+DY(i)+2.*DY(i))
134 |40 continue
135 |41 RETURN
136 |6 END
137 |7 Subroutine Deriva(KH,YT,DYDX)
138 |8 dimension dydx(4), yt(4)
139 |9 implicit double precision (a-h,o-z)
140 |0 ex=yt(2)/(yt(2)**2+2*yt(1)**2)**(3.0/2.0)
141 |1 ey=yt(1)/(yt(2)**2+2*yt(1)**2)**(3.0/2.0)
142 |2 c sqrt(ex**2+ey**2)
143 |3 w=1000.0
144 |4 c b=137.0/2.0
145 |5 c b=30.0
146 |6 c b=10.3463
147 |7 c b=10.1234
148 |8 c b=30.0
149 |9 c define diff eq
150 |0 dydx(1)=yt(3)
151 |1 dydx(2)=yt(4)
<table>
<thead>
<tr>
<th>Line</th>
<th>Code</th>
</tr>
</thead>
<tbody>
<tr>
<td>153</td>
<td>dydx(3) = (2.0/137.0) * b * yt(4) - ey</td>
</tr>
<tr>
<td>154</td>
<td>dydx(4) = (2.0/137.0) * b * yt(3) - ex</td>
</tr>
<tr>
<td>155</td>
<td>dydx(3) = wo * yt(4) - ey</td>
</tr>
<tr>
<td>156</td>
<td>dydx(4) = wo * yt(3) - ex</td>
</tr>
<tr>
<td>157</td>
<td>return</td>
</tr>
<tr>
<td>158</td>
<td>end</td>
</tr>
</tbody>
</table>
APPENDIX 3

PROGRAM TO GENERATE THE DATA FOR THE BIFURCATION GRAPHS.

This program was used to generate the data for the bifurcation diagrams for the Logistic equation and Equations 2.2 through 4.1 on pages 25-26 of the thesis.
1. x=0.65
2. n=148
3. a=2.775
4. do 20 l=1,n
5. if(a.lt.24) then
6. a=a+.025
7. endif
8. do 10 j=1,100
9. x=a*x*(1-x)
10. if(j.gt.980) then
11. write(*,*)a,x
12. else
13. endif
14. continue
15. continue
16. end
APPENDIX 4

DUFFING OSCILLATOR PROGRAM.

This program was used to generate the phase space diagrams for the forced damped pendulum and the undamped pendulum.
c driver for rk dumb
c this is xvl7.f
ct The check program for xvl7.f is casave.f but wo(frequency)
c must be adjusted to match the (xvl7.f) frequency.
c
parameter(nvar=2,nstep=1024)
do
common /path/x(1024),y(2,1024)
de
implicit double precision (a-h,o-z)
do
external deriv
do
x1=0.0
no
x1 is the initial time.
oc
not that all x-variables are for time.also xt,xh,x+h in rkg.
do
vstart(1)=1.5
do
vstart(2)=0.1
do
vstart(3) is x1
do
vstart(2) is dxl/dc
do
x2=30.0
no
x2 is the final time.
do
call rk dumb(vstart,nvar,xt,x2,nstep,derivs)
do
10 i=1,nstep
do
write(6,*),y(1,i),y(2,i)
do
continue
do
stop
do
end
SUBROUTINE RK DUMB (VSTART, NVAR, XI, X2, NSTEP, DERIVS)
do
PARAMETER (NMAX=2)
do
COMMON /PATH/ XX(NVAR), Y(NVAR)
de
implicit double precision (a-h,o-z)
do
DIMENSION VSTART(NVAR), V(NVAR), DV(NVAR)
do
DO 11 I=1,NVAR,1
do
V(I)=VSTART(I)
do
XX(1)=XI
do
XX(I+1)=XI
do
H=(X2-X1)/NSTEP
do
DO 13 I=1,NSTEP,1
do
CALL DERIVS (X,V,DV)
do
CALL RK4 (V,DV,NVAR,X,H,V,DERIVS)
do
IF(X+H.EQ.X>PAUSE 'Stepsize not significant in RK DUMB.'
do
XX(I)=XI
XX(I+1)=XI
DO 12 I=1,NVAR,1
do
IF(X.I.EQ.X) GOTO 10
ndo
10 CONTINUE
ndo RETURN
endo
END
SUBROUTINE RK 4 (y, DYDX, N, X, H, YOUT, DERIVS)
do
PARAMETER (NMAX=4)
do
DIMENSION Y(NVAR), DYDX(NVAR), YOUT(NVAR), DY(NVAR), DTY(NVAR)
de
implicit double precision (a-h,o-z)
do
HH=H*0.5
ndo
HH=H/6.
do
XH=X+HH
ndo
DO 12 I=1,NVAR,1
do
Y(I)=Y(I)+HH*DYDX(I)
do
12 CONTINUE
ndo RETURN
endo
END
SUBROUTINE DerIVs(XT,YT,DYDX)
do
dimen son dydx(4), yt(4)
do

IMPLICIT DOUBLE PRECISION (A-H,O-Z)

DEFINE DIFF EQ

F=2.0
d=.015
w=1.0

 dydx(1) = y(2)
dydx(2) = -d*y(2)*y(1)-y(1)**3+f*cos(w*x)

RETURN
END
APPENDIX 5

ERROR CORRECTION PROGRAM.

This program was an attempt at correcting for possible rounding and truncation error which develops as the time the program runs for is increased.
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1: I drive
2: I this is cv17.f
3: I parameter(nvar=6,nstep=1000)
4: I dimension vsstart(4)
5: I common /path/xp(1001),yp(4,1001),kmax,kount,dxav
6: I implicit double precision (a-h,o-z)
7: I real M,q-xl,x2,x3,x4,x5,x6
8: I x1=0.0
9: I x is initial time
10: I note that all x-variables are for time also xt,xh,x+h in rk4.
11: I note!!!! Increase the array size for nstep, to make nstep smaller.
12: I I did this in xv300.f
13: I vsstart(1)=0.1
14: I vsstart(2)=0.0
15: I *making velocity smaller so can get x=3.0,y=1.0 to
16: I *orbit had Vy=0.5
17: I * vsstart(1)=1.0
18: I * vsstart(2)=0.0
19: I * vsstart(4) = vx
20: I * vsstart(3) = vy
21: I * vsstart(1) = y(t)
22: I * vsstart(2) = x(t)
23: I * x2=1000.0
24: I x2=50.0
25: I ****???calculate energy in atomic units*******
26: I q=1.0
27: I q=3.0
28: I x2 is the final time
29: I call vxdumb(vsstart,nvar,xl,x2,nstep)
30: I **nob,nbed)
31: I DO 9 1=1,nstep
32: I y(i,1)=vsstart(i)
33: I DO 13 k=1,nstep
34: I y(i,k+1)=ysstart(i)
35: I DO 10 1=1,nstep
36: I v(t)=sqrt(y(4,1)**2+y(3,1)**2)
37: I r=sqrt(y(1,1)**2+y(2,1)**2)
38: I t=(u/2.0)*v(t)**2-q**2/r
39: I write(6,*)y(i,1),y(i,1)
40: I write(6,*)y(i,2,1),y(i,1)
41: I DO 12 continue
42: I DO 10 continue
43: I DO 10 1=1,nstep
44: I vt=sqrt(y(4,1)**2+y(3,1)**2)
45: I z=sqrt(y(1,1)**2+y(2,1)**2)
46: I t=(-u/2.0)*y(2,1)**2-y(3,1)**2-q**2/z
47: I write(6,*)y(4,1),y(3,1)
48: I write(6,*)y(4,1),y(3,1)
49: I write(6,*)y(4,1),y(3,1)
50: I write(6,*)y(4,1),y(3,1)
51: I n2=n2+1
52: I if (n2.eq.50) then
53: I write(6,*)time energy x(t)
54: I endif
55: I write(6,*)x(i),y(j,1),y(j,1)
56: I n2=0
57: I endif
58: I write(6,*)
59: I write(6,*)
60: I write(6,*)
61: I write(6,*)
62: I endif
63: I continue
64: I stop
65: I end
66: I
drive
67: I
drive
68: I
drive
69: I
drive
70: I
drive
71: I Subroutine derivs(XT,YT,DYDX)
72: I dimension dydx(4),yr(4)
73: I common /path/ xp(1001),yp(4,1001),kmax,kount,dxav
74: I real b,ex,ey,wo
75: I implicit double precision (a-h,o-z)
76: I b=50.0
we can calculate the energy to determine if the orbit is closed or if energy is negative. It appears that this energy equation has nothing to do with the below equations since there is no $V_x$ and $V_y$ in the Lorentz equation below, but this program is calculating $V_x$ and $V_y$ which are used in the energy equation and therefore dependent.

**DEFINE DIFF EQ**

```
dydx(1) = yt(3)
dydx(2) = yt(4)
dydx(3) = -wo*yt(4)
dydx(4) = wo*yt(3)
return
end
```

**SUBROUTINE RK4(VSTART, NVAR, XI, X2, NSTEP)**

```
PARAMETER (NMAX=4)
COMMON /PATH/ X(X(1001), Y(4,1001))
DIMENSION VO START(NVAR), V(NMAX), DV(NMAX)
DO 11 1=1, NVAR, 1
V(I) = VSTART(I)
K(1) = 1, NSTEP, 1
CALL DERIVS(X, V, DV)
CALL RK4(V, DV, NVAR, X, H, V)
IF(X+H.EQ.X)PAUSE 'Step size not significant in REDMBS.'
X=X+H
DO 12 1=1, NSTEP, 1
YT(I)*YT(I)+HH*DYDX(I)
CONTINUE
CALL DERIVS(XH, YT, DYT)
DO 12 1=1, NSTEP, 1
YT(I) = YT(I)+HH*DYT(I)
CONTINUE
CALL DERIVS(XH, YT, DYM)
DO 13 I=1, NSTEP, 1
YT(I) = YT(I)+HH*DYM(I)
CONTINUE
RETURN
END
```

**SUBROUTINE RK4(V, DYDX, N, X, H, YOUT)**

```
PARAMETER (NMAX=4)
COMMON /PATH/ XP(1001), YP(4,1001), KMAX, KOUNT, DXAV
DIMENSION X(N), DYDX(N), YOUT(N), YT(NMAX), DYT(NMAX), DYM(NMAX)
COMMON /path/ XP(1001), YP(4,1001), KMAX, KOUNT, DXAV
DIMENSION X(N), DYDX(N), YOUT(N), YT(NMAX), DYT(NMAX), DYM(NMAX)
COMMON /path/ XP(1001), YP(4,1001), KMAX, KOUNT, DXAV
DIMENSION X(N), DYDX(N), YOUT(N), YT(NMAX), DYT(NMAX), DYM(NMAX)
```

```
do 11 1=1, 4
yt(1) = yt(1)+hh*dydx(1)
do 11 1=1, 4
yt(2) = yt(2)+hh*dydx(2)
do 11 1=1, 4
yt(3) = yt(3)+hh*dydx(3)
do 11 1=1, 4
yt(4) = yt(4)+hh*dydx(4)
do 11 1=1, 4
xt(1) = xt(1)+hh*dxav
xt(2) = xt(2)+hh*dxav
xt(3) = xt(3)+hh*dxav
xt(4) = xt(4)+hh*dxav
```

```
RETURN
END
```
Subroutine rkqc(Y, DYDX, N, XTTRY, EPS, YSCALE, MIDG, HNEXT)

parameter (nmax=4, pgrow=-0.20, pshrink=-0.25, fcorr=1.0/15.0, 
* one=1.0, safety=0.9, ermaxc=6.0e-4)

c common /path/xp(1001), yp(4,1001), kmax, kount, dxsav

dimension y(n), dydx(n), yscal(n), ytemp(nmax), ysav(nmax), 
* dysav(nmax)

xsav=x

do 11 1=1,n

ysav(i)=y(i)
dysav(i)=dydx(i)

continue

h=0.5*h

call rk4(ysav, dysav, n, xsav, hh, ytemp)
x=xsav+hh
call derivs(x, ytemp, dydx)
call rk4(ytemp, dydx, nh, hh, y)

11 continue

h=htry

if(x .eq.xsav) pause 'stepsiz not significant in rkqc'
call rk4(ysav, dysav, n, xsav, b, ytemp)

errmax=0.0

do 12 1=1,n
ytemp(i)=y(i)-ytemp(i)

errmax=max(errmax, abs(ytemp(i)/yscal(i)))

12 continue

errmax=errmax/eps

if(errmax, qf, one) then

h=safety*h*(errmax**pshrink)
go to 1
else

hdid=h

if(errmax, qf, ermaxc) then

hnext=safety*h*(ermaxc**pgrow)
else

hnext=4.0*h

endif

200 endif

201 do 13 1=1,n

y(i)=y(i)+ytemp(i)*fcorr

13 continue

204 return

205 end

SUBROUTINE ODIENT(YSTART, nvar, X1, X2, EPS, HI, HBEG, HOK, HBAD)

parameter (maxstp=1000, nmax=4, two=2.0, zero=0.0, tiny=1.0e-30)

c common /path/ xp(1001), yp(4,1001), kmax, kount, dxsav

dimension ystart(nvar), yscal(nmax), y(nmax), dydx(nmax)

kmax=15

dxsav=10

x=x1

h=sign(h1, x2-x1)
nok=0

nbad=0

kount=0

do 11 1=1,nvar

y(i)=ystart(i)

11 continue

if(kmax, qf, 0) xsav=x-dxsav*two

do 16 nstp=1, maxstp

call derivs(x, y, dydx)

do 22

16 continue

22 do 12 1=1,nvar

12 continue
229:           yscal(i)=abs(y(i))+abs(h*dydx(i))+tiny
230:          continue
231:          if(kmax.gt.0) then
232:              if(abs(x-xsav).gt.abs(dxsav)) then
233:                  if(kount.lt.kmax-1) then
234:                      kount=kount+1
235:                      xp(kount)=x
236:                      do 13 1=1,nvar
237:                          yp(1,kount)=y(1)
238:                      13 continue
239:                      x.sav=x
240:                      endif
241:                      endif
242:                      endif
243:              if((x+h-x2)*(x+h-x1).gt.zero) then
244:                  call rkq(y,dydx,nvar,x,h,eps,yscal,hdid,hnext)
245:                  if(hdid.eq.hthen)
246:                      nok=nok+1
247:                  else
248:                      nbad=nbad+1
249:                      endif
250:              if((x-x2)*(x2-x1).ge.zero) then
251:                  do 14 1=1,nvar
252:                      ystart(i)=y(i)
253:                  14 continue
254:              if(kmax.ne.0) then
255:                  kount=kount+1
256:                  xp(kount)=x
257:                  do 15 1=1,nvar
258:                      yp(1,kount)=y(1)
259:                  15 continue
260:              endif
261:              return
262:          endif
263:          endif
264:          if(abs(hnext).lt.hmin) pause 'stepsize smaller than minimum'
265:          h=hnext
266:          continue
267:          pause 'to many steps'
268:          return
269:          end
APPENDIX 6

LYAPUNOV EXPONENT PROGRAM.

This program was an attempt at calculating and understanding the methods for the calculation of the Lyapunov exponent.
```fortran
1 dimension y(12), znorm(3), gac(3), cum(3), ynew(12)
2 external function
3 common ypml
4
5 nn=12
6 y(1)=0.5
7 y(2)=0
8 y(3)=0.46666667
9 do 1 =nn,1,1
10 y(i)=0.0
11 continue
12 do 10 =1,nn,1
13 continue
14 continue
15 continue
16 continue
17 continue
18 continue
19 do 10 =1,nn,1
20 y(1)=0.0
21 y(2)=0
22 if(y(3).lt.2*(3.14)*numorbit) then
23 call zkk4(y,nn,tstep,q,w,g,ynew)
24 continue
25 do i=1,nn,1
26 y(k)=ynew(k)
27 continue
28 continue
29 do 10 =1,nn,1
30 znorm(1)=znorm(1)+y(n*k+1)**2
31 continue
32 continue
33 continue
34 continue
35 continue
36 continue
37 continue
38 gac(1)=0.0
39 do 10 =1,nn,1
40 gac(i)=gac(i)+y(n*k+1)*y(n*k+1)
41 continue
42 continue
43 do 20 =1,nn,1
44 znorm(j)=znorm(j)+y(n*k+1)**2
45 continue
46 continue
47 continue
48 do 20 =1,nn,1
49 znorm(j)=znorm(j)+y(n*k+1)*y(n*k+1)
50 continue
51 continue
52 continue
53 continue
54 continue
55 cum(k)=cum(k)+log(znorm(k))
56 print*I,***I think above is the total of the lyapunov exponents***
57 continue
58 if(y(3).le.0) then
59 cum(k)/=cum(k)/c
60 write(6,'*cumk')
61 continue
62 continue
63 continue
64 end if
65 end
66 end
67 subroutine zkk4(y,nn,tstep,q,w,g,ynew)
68 dimension y(12), y2(12), y3(12), y4(12), y5(12), y6(12), y7(12), y8(12), y9(12)
69 *ynew(12), y(12)
70 common ypml
71 write(6,'*two')
72 continue
73 do 60 =1,nn,1
74 y(k)=tstep*ypml(y,k,q,w,g)
75 print*I,***the program has problems right here*************
76 continue
77 print*I,there is a problem with the function routine**********
```
```fortran
78 | write(6,'*')
79 | continue
80 | do 65 k=1,nn,
81 | write(6,'*')
82 | y1(k)=y(k)-y1(k)/2
83 | continue
84 | do 70 k=1,nn,
85 | y2(k)=step*ypirim(yy1,k,q,w,g)
86 | continue
87 | do 75 k=1,nn,
88 | yy2(k)=y(k)+y2(k)/2
89 | continue
90 | do 80 k=1,nn,
91 | y3(k)=step*ypirim(yy2,k,q,w,g)
92 | continue
93 | do 85 k=1,nn,
94 | y3(k)=y(k)+y3(k)
95 | continue
96 | do 90 k=1,nn,
97 | y4(k)=step*ypirim(yy3,k,q,w,g)
98 | continue
99 | do 95 k=1,nn,
100 | ynew(k)=y(k)+y1(k)+2*y2(k)+2*y3(k)+y4(k)/6
101 | return
102 | end
103 | end
104 | function ypirim(y,k,q,w,g)
105 | dimension y(12)
106 | common /ypirim/
107 | if(k.eq.1) then
108 | ypirim=-y(1)/q-y(2)+g*cos(y(3))
109 | end if
110 | if(k.eq.2) then
111 | ypirim=y(1)
112 | end if
113 | if(k.eq.3) then
114 | ypirim=w
115 | end if
116 | if(k.gt.3) then
117 | if(k.gt.6) then
118 | k=k-6
119 | ypirim=y(4+1)/q-y(7+1)*cos(y(2))+y(10+1)*sin(y(3))
120 | end if
121 | end if
122 | if(k.gt.6) then
123 | if(k.gt.10) then
124 | k=k-7
125 | ypirim=y(4+1)
126 | end if
127 | end if
128 | if(k.gt.9) then
129 | ypirim=0
130 | end if
131 | return
132 | end
```
BIBLIOGRAPHY


