A Classical Approach to the Stark-Effect

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Abstract

The state of an atom in the presence of an external electric field is known as a Stark state. For constant fields, electrons in a Stark state of various Rydberg atoms of Lithium have been found to exhibit chaos for certain values of energy and strength of the electric field. In this paper we study this phenomenon from a classical point of view for the Na Rydberg atom, in an effort to determine the set of physical conditions for which the Stark system of this atom exhibits core-induced chaos.

1. Introduction

1.1 A brief description

The energy levels of an atom change when the atom is subjected to an external electric field. This effect is known as the classical Stark effect. Although this effect has been explained in great detail quantum mechanically, the behavior of the system for certain physical conditions has been found to be quite unpredictable. More precisely, by varying parameters of the system, like the strength of the electric field and initial conditions of the electron including its energy and classical momentum, chaotic behavior for the electron has been found. Outer electrons with low angular quantum number ($l < 3$) have orbits that penetrate the core consisting of the nucleus and the inner electrons, and this core interaction has been found to induce chaos in the system. This paper attempts to analyze such behavior for the Na Rydberg atom.

1.2 Motivation

In quantum mechanics, the Stark effect is approached by using the fundamental Schrödinger equation:

$$ih \frac{\partial \psi}{\partial t} = \left( -\frac{\hbar^2}{2m} \nabla^2 + V \right) \psi$$

However, an important observation in the above equation is that it is linear in the wave function $\psi$. This eliminates chaotic behavior for the system since nonlinear equations governing the system are a necessary condition for chaos [1]. Systems in classical mechanics, however, are very often governed by nonlinear equations. This is the reason one turns to classical mechanics in an effort to analyze chaotic behavior. The classical approach is not always correct, while the quantum
mechanical approach is always correct. One reason why the classical approach is reasonable in this case is because we are analyzing Na Rydberg atoms. These are Na atoms with the outermost valence electron in very highly excited states, with principal quantum number \( n > 20 \). This puts the system in the correspondence zone between classical and quantum mechanics, thus justifying the classical approach.

The goal then in studying such “chaotic” systems classically is to develop a new quantum mechanical approach to characterizing such systems.

2. Chaotic behavior

2.1 Definitions

In order to analyze the problem at hand, we first define the framework and methods of analysis which will be used. A dynamical system is said to be chaotic if it exhibits extremely sensitive dependence to initial conditions. Quantitatively, let \( \alpha \) and \( \alpha + \varepsilon \) be two different initial conditions of a system, where \( \varepsilon \) is extremely small. Let \( X_\alpha \) and \( X_{\alpha + \varepsilon} \) represent the states of the system which evolve after time \( t \), starting with initial conditions \( \alpha \) and \( \alpha + \varepsilon \) respectively. Then the two states \( X_\alpha \) and \( X_{\alpha + \varepsilon} \) might be entirely different even for very small \( \varepsilon \). It is important to note that chaotic behavior is different from random behavior in that the chaotic behavior is deterministic. This means that the state of the system at some time \( t_k \) can be computed from the state of the system at time \( t_{k-1} \). However, the state of the system cannot be computed for some later time \( t_j (j \gg k) \) because the system is very sensitive to initial conditions and a small uncertainty of \( \Delta x \) in these conditions could affect the state at \( t_j \) drastically. As mentioned earlier, a necessary condition for chaotic behavior is nonlinearity in the system. From now on, we will assume the given system to be nonlinear unless otherwise mentioned.

2.2 Deterministic analysis

2.2.1 Maps: Phase space and Poincaré maps

The first step in analyzing a given system governed by certain differential equations is to obtain from these a set of difference equations. A difference equation is an equation whose variables take on discrete values so that our problem is reduced to observing the system at discrete time intervals. Hence a continuous time equation of the form \( \frac{dx}{dt} = -kx^2 \) reduces to a difference equation of the form \( x_{n+1} = x_n + \alpha(-kx_n^2) \) where \( \alpha \) is a constant. Therefore a difference equation is of the form \( x_{n+1} = f(x_n) \). Thus we obtain equations of state which give us a deterministic behavior as discussed before. Now, since the system at any given time is uniquely determined by the preceding state of the system, if the system ever repeats a state with the same characteristics, the motion is periodic. This is the basis of phase space analysis. For a system with 1 degree of freedom \( x \),
the characteristics which define the system completely are \( x \) and \( \dot{x} \). Therefore we plot the system’s trajectory in the \( \dot{x}-x \) plane and obtain a phase plane (we use space for 3 dimensions or more, plane for 2 dimensions). Then clearly, a periodic motion in this system is characterized by a closed orbit in the phase plane.

A phase space for a system having \( n \) degrees of freedom is a space of \( 2n \) dimensions, representing the velocity and magnitude of each degree of freedom. A complicated, incomplete trajectory in the phase space implies chaos. Phase spaces though are often hard to use in the case of complicated trajectories, or when the number of degrees of freedom is large. Here is where we introduce the idea of Poincaré maps.

A Poincaré map is obtained from phase space by taking coordinate sections of the space. An example of a Poincaré map is obtained by observing values of \( x \) and \( \dot{x} \), by taking sections of the phase space \( (\dot{x}-x) \) at regular time intervals. This increases the clarity in the phase space since a closed orbit in phase space would map to just a set of points in the Poincaré map. By choosing the values of the fixed coordinate appropriately, the clarity of the Poincaré map can be improved. For example, for a pendulum, upon choosing the time interval between fixed values of time \( (t_n - t_{n-1}) \) to be the time period of oscillation, the Poincaré map will consist of only one point when the pendulum is perfectly periodic. Some thought reveals that finite, discrete points in the Poincaré map reflect periodic orbits while complicated maps with fractal like appearances reflect chaotic behavior. However, like the phase space, this map also increases in complexity very fast with an increase in the number of degrees of freedom. Hence, for systems involving 3 or more degrees of freedom, Poincaré maps associated with each degree of freedom are studied, holding the other degrees of freedom fixed, or varying them discretely. So for a problem having 3 degrees of freedom, say \( (x, y, z) \), one Poincaré map which is studied is the \( \dot{x} - x \) plane obtained by holding \( y \) and \( z \) constant at some value(s). Similarly, maps can be obtained by holding pairs of variables \( x \) and \( z \), and \( x \) and \( y \) constant.

As an application, let us consider the driven, damped pendulum as shown above. In figure 2, we analyze the above system for different values of the force \( F \), using phase planes and Poincaré maps. In the analysis [1], the left column gives us the angular velocity versus time, the center column shows the phase plane \( (\dot{\theta}, \theta) \), and the right column the Poincaré map for the system. We note the
system’s behavior for different values of the driving force. In the first case the system is perfectly periodic and a closed trajectory in the phase plane indicates this very clearly. In the second case \((F = 0.5)\), the system again has a closed orbit but this time finite points on the Poincaré map are a better indicator of the periodicity. For the \(F = 0.6\) case, the fact that the system is chaotic is seen clearly in the phase plane.

Figure 2: Analyzing systems using phase planes and Poincaré maps [1]

2.2.2 Bifurcation Diagrams

To facilitate explanation of this section, we consider a 1 dimensional system described by variable \(x\) and having certain initial condition \(\alpha\). Now for a given \(\alpha\), \(x_n\) evolves in time to form a certain orbit so that there are discrete values which \(x_n\) takes. As \(\alpha\) is changed, this set of values changes. A bifurcation diagram is one which plots possible values of \(x_n\) against different values of \(\alpha\). As the system approaches chaos due to changes in initial parameters \((\alpha)\), we find the domain of \(x_n\) increasing and finally, in a chaotic state, \(x_n\) can vary over the whole domain for the given \(\alpha\). Thus by looking at how the domain of the state variables describing the system changes for different initial conditions, we can determine which initial conditions bring about a chaotic system. As an example, we analyze a system given by the difference equation

\[
x_{n+1} = \alpha x_n (1 - x_n)
\]

The bifurcation diagram obtained for the above system is shown in figure 3. By iterating the above
function few times, we see that for $\alpha < (\approx 3.1)$, the system always converges to a fixed point (where $x_{n+1} = x_n$). This is seen in the bifurcation diagram as a single line for $\alpha < (\approx 3.1)$. For $(\approx 3.1) < \alpha < (\approx 3.45)$, the system is in a two point equilibrium. Again, the bifurcation diagram reflects this by showing two values of $x_n$ for each $(\approx 3.1) < \alpha < (\approx 3.45)$. From the bifurcation diagram then, the system exhibits chaos for values of $\alpha$ greater than approximately 3.57 since $x_n$ now span the entire range and does not converge to any given set. However, there are intermittent values of $\alpha$ in this range where the system suddenly goes periodic (where the bifurcation set for $x_n$ again becomes a finite number of points).

Figure 3: Bifurcation diagram for $x_{n+1} = \alpha x_n (1 - x_n)$ [1]

3. Orbital Dynamics of the Stark System

We now return to the Stark system in order to determine the nature of the electron orbits in an atom, using the methods of analysis mentioned in section 2. To observe the orbit of an electron classically, we use Lagrange’s equations of motion [1] given by

$$\frac{\partial L}{\partial x_i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}_i} = 0$$

(1)

where $x_i$ are the coordinates of the particle and $L$ the Lagrangian for the particle. Since the equations of motion for an electron in the Stark system are not solvable analytically, numerical integration methods are used to compute the orbit of the electron. A detailed description of Lagrange’s equations of motion for the Stark system and the numerical methods used in solving them is given in the Appendix. It is important to note that all our analysis is in atomic units (Table 1). Atomic units are defined so that all the relevant parameters (except energy) for the ground state of hydrogen have a magnitude of 1 (the energy in atomic units is $-1/2$).
Table 1. Atomic Units. For a more detailed description, see Bethe and Salpeter [6].

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Atomic Units</th>
<th>CGS units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time</td>
<td>1</td>
<td>$2.4189 \times 10^{-17}$ sec.</td>
</tr>
<tr>
<td>Length</td>
<td>1</td>
<td>$5.2917 \times 10^{-9}$ cm.</td>
</tr>
<tr>
<td>Energy</td>
<td>1</td>
<td>$4.359 \times 10^{-11}$ erg.</td>
</tr>
<tr>
<td>Electric Field</td>
<td>1</td>
<td>$5.142 \times 10^{9}$ V/cm.</td>
</tr>
</tbody>
</table>

3.1 The Runge-Lenz Vector

For the classical orbit of an electron in an atom, we can define the Runge-Lenz vector $\mathbf{A}$ as follows:

$$\mathbf{A} = \mathbf{p} \times \mathbf{L} - \hat{r}$$

where $\mathbf{p}$ is the linear momentum, $\mathbf{L}$ the total angular momentum and $\hat{r}$ the unit vector in the direction of the displacement vector $\mathbf{r}$ (all in atomic units). The Lenz vector thus is always in the plane of the orbit and in the case when the potential is of the form $1/r$ (so that the orbit is a closed ellipse), the Lenz vector points to the pericenter (point of closest approach to the nucleus) of the orbit [7]. Further, it can be shown that both the magnitude and the direction of the Lenz vector are constants of motion when the potential is of the form $1/r$ [7]. We shall refer to the Lenz vector in later sections and in the Appendix.

3.2 Orbits without electric fields

In order to observe and identify chaotic orbits, it is necessary for us to be well acquainted with orbit maps and diagrams in the absence of chaos. We therefore begin our analysis by observing orbits in the absence of electric fields. We first look at the electron orbits observed in the Hydrogen Rydberg atom. We look at the (principal quantum number) $n = 10$ state for the Hydrogen atom, which is a Rydberg state [5]. Since the potential for the atom is of the form $1/r$, we obtain elliptical orbits, the eccentricity of which are determined by the azimuthal quantum number $l$. Figure 4 below displays the orbit of the electron in real space (cartesian co-ordinates) for the case $l = 9$.

The orbit is almost completely circular, since the eccentricity, given by $\sqrt{1 - l(l + 1)/n^2}$, is almost 0. As $l$ is reduced, the eccentricity of the orbit increases and the orbit for $l = 1$ is shown in figure 5.

It is important to note here some differences in the classical and quantum mechanical treatment of this problem. Although quantum theory allows an $l = 0$ state, classically this corresponds to a state where $L = \sqrt{l(l + 1)} = 0$, which implies an orbit without any angular momentum. Classically, such an orbit does not exist and hence this state is excluded from our analysis.

As the atomic number $Z$ is increased however, for small $l$ it becomes necessary to modify the $1/r$ potential. This can be seen in figure 6. For an orbit with high eccentricity (low $l$), the
outer electron comes very close to the nucleus. In the case of the hydrogen atom, the nucleus is a point charge and hence the potential still remains $1/r$, however, for larger atoms, this results in the electron penetrating the core (see figure 6 below) which changes the form of the potential. This modification of the potential results in the observance of quantum defects [5].

Hence, for a Na Rydberg atom ($Z = 11$), when working with low $l$, it is convenient to model the potential to a form given by [3]

$$V(r) = -\frac{1}{r} - \frac{(Z-1) e^{-\alpha r}}{r}$$

(2)

where $\alpha$ is chosen to give the best agreement with measured quantum defects. Such a potential no longer allows closed elliptical orbits, but produces orbits as shown in figure 7 below, where the precession of the elliptical orbit is related to the quantum defect $\delta_l$ by

$$\theta(\alpha) = 2\pi \delta_l$$
where $\theta(\alpha)$ is the angle of precession of the orbit corresponding to $\alpha$.

Although the fact that this orbit is not chaotic is clear from viewing the real space, it is instructive to observe the phase space for the orbit. However, the phase space plots for these orbits are observed not in cartesian coordinates, but in semi-parabolic coordinates. The reason is that while in cartesian coordinates the potential has a singularity at the origin, semi-parabolic coordinates eliminate this singularity [8]. Semi-parabolic coordinates $(u, v, \phi)$ are defined as follows:

$$u = (r + z)^{1/2}, \quad v = (r - z)^{1/2}, \quad \phi = \arctan \frac{y}{x}$$

where $x$, $y$ and $z$ are cartesian coordinates and $r = (x + y + z)^{1/2}$. The phase space plot for the orbit in figure 7, in semi-parabolic coordinates is shown below in figure 8.

3.3 Computation of $\alpha$ in $V(r)$
Before computing the various real space and phase space maps for the Na Rydberg atom, it is necessary for us to compute the parameter $\alpha$ in equation (1). Since the quantum defects $\delta_l$ for the Na Rydberg atom are known, the value of $\alpha$ can be determined by measuring the angle of precession. We computed the value of $\alpha$ which agreed with the quantum defects $\delta_s$ and $\delta_p$ of the $n = 27$ state of the Na Rydberg atom. The values for these defects used were $\delta_s(27) = 1.24806$ and $\delta_p(27) = 0.854789$ [5]. By varying $\alpha$ and using a program to compute the angle of precession from the orbit corresponding to $\alpha$, we found that at $\alpha = 2.625$,

$$\theta(\alpha) = 2\pi\delta_s(27) \pm 0.03$$

for the s state and

$$\theta(\alpha) = 2\pi\delta_p(27) \pm 0.01$$

for the p state. This agreement is sufficient for our purposes due to the high frequency of chaos that has been predicted in the Na Rydberg system by observing the Li Rydberg system [4]. All further calculations were made using this value of $\alpha$.

### 3.4 Orbits in the presence of an external electric field

The introduction of a constant external electric field changes the form of the potential and thus the electron’s orbit. For convenience of analysis, we shall apply the constant electric field perpendicular to the plane of the orbit, so that perturbations in the orbit due to the field can be distinguished from core potential precessions. In our analysis, the orbit is kept in the $x$-$y$ plane.
and the electric field is applied in the $+z$ direction. Therefore the potential assumes the form

$$V(r) = -\frac{1}{r} - \frac{(Z-1)e^{-\alpha r}}{r} + Fz$$

where $F$ is the constant electric field and the other variables are the same as in equation (2).

We first observe the real space orbit of the hydrogen atom in the presence of an electric field. Figure 9 below shows the real space orbit for the hydrogen atom in the $n = 10$, $l = 1$ state with $F = 0.0625 \times 10^{-6}$ au. Although the real space orbit does reveal a new orbit, a comparison of the Phase space plots in figure 10 shows the change more clearly. However, it is known that the hydrogen atom does not exhibit chaos in the presence of an electric field. This is seen by the sharply defined regions in phase space in figure 10, where as a chaotic phase space has undefined boundary regions in phase space (see figure 15). Further, the orbits in a chaotic state fill up the phase space completely, where as the orbits in the hydrogen atom cover only a definite restricted region of the phase space (figures 10).

Figure 9: Real Space Plot for the H Rydberg atom with an electric field, in cartesian coordinates, $n = 10$, $l = 1$. Field strength $F = 0.0625$ au.

This periodic behaviour however, is lost in the case of the Na Rydberg atom. We first look at the case without electric fields. Figure 11 shows clearly the difficulty in reading real space plots and hence we restrict our analysis to phase space plots. Figure 12 (same as figure 9) shows the phase space plot (in semi-parabolic coordinates) for the Na Rydberg atom without an electric field. The map shows very clearly the periodic behaviour of the electron.

As the field strength is increased, the orbit begins to precess in the $z$ direction as well, and the resultant phase space plots are shown in figure 13 for field strengths $F = 0.3$ au and $F = 0.45$
au. A single precession in the orbit was observed after the system evolved for about (time=) 2 au. The orbits in figures 12 and 13 were allowed to evolve for about (time=) 400 au before a plot was obtained. The orbits in figure 13 are not chaotic, by a similar argument as before, that is the phase space plots in both cases contained very well defined restricted regions. Also, a small change in the value of the field did not affect the phase space plots obtained, showing no sensitive dependence on $F$, a prerequisite for chaos.

As the field was increased to beyond 0.5 au, the orbit showed signs of unstable behaviour. At $F = 0.521080$ au, the phase space plot strongly suggested chaotic behaviour. This is shown in figure 14. This was further strengthened by the observance of distinctly different phase plots for small changes in the field (sensitive dependence on $F$). These are shown in figure 15, where phase plots for $F = 0.521075$ au and $F = 0.521085$ au are shown. Also, the system became excessively chaotic after it had evolved for about (time=) 200 au in each of the above cases, so that the numerical integrator could no longer compute the orbit successfully (minimum machine stepsize was reached).

We also plotted the bifurcation diagram for the Na Rydberg Stark system for field strengths around $F = 0.52$ au. Figure 16 shows the bifurcation plot for the system obtained by varying the field strength from $F = 0.5205$ au to $F = 0.5235$ au. The system was let to evolve for (time=) 50 au and the coordinates of the electron were observed every (time=) 2 au. The distinct perturbation in the diagram at $F \approx 0.5208$ again strongly suggests chaotic behaviour in that region.

4. Results and Conclusion
By observing the precession of the Na Rydberg atom in the $n = 27, l = 1$ state and comparing it to known quantum defects, we found a fit to the core potential to use for our analysis. We also found strong evidence that the Na Rydberg Stark system exhibits chaotic behaviour for certain system parameters. The orbital analysis in section 3 was done in great detail for the atom in the $n = 27, l = 1$ state with $F = 0.52018$ au. We found that phase plots obtained at the above mentioned regime showed very sensitive dependence on the field strength. The phase plots consisted of regions having undefined boundaries, which covered most of the phase plane. The bifurcation diagram also suggested chaotic behaviour in the region $F \approx 0.52018$. All three results strongly suggest chaotic behaviour for the Na Rydberg atom in the $n = 27, l = 1$ state with electric field $F = 0.52018$ au.

However, in cgs units, this electric field corresponds to a colossal $2.67 \times 10^9$ V/cm. It is known however, that (assuming no Stark shifts) the electric field needed to ionize an electron within an atom is given by $F_n = \frac{1}{16n^2}$ au (where $n$ is the principal quantum number). For $n = 27$, this corresponds to an ionization field strength of about $0.117 \mu$ au or 604.7 V/cm. This calculation clearly shows an error in the value of the chaotic field strength of $2.67 \times 10^9$ V/cm obtained in section 3. We believe that this is due to the value chosen for the parameter $\alpha$ in the core potential (2). It is concluded that the method of using the angle of precession to compute $\alpha$ is incorrect for larger atoms like Na (it was found suitable for Li), and some other methods must be used to compute an acceptable value for $\alpha$. A crude approximation can be obtained by varying $\alpha$ so that exponential term $\frac{(Z-1)e^{-\alpha r}}{r}$ decreases to an insignificant fraction of the $1/r$ term (2) when $r$ is
Figure 12: Phase Space Plot for the Na Rydberg atom with no electric field, in semi-parabolic coordinates $\dot{u}-u$, $n = 27$, $l = 1$.

approximately equal to the radius of the core. Subsequently, a similar analysis as the one shown in section 3 can be performed. We intend to pursue this analysis in the near future.
Figure 13: Phase Space Plots for the Na Rydberg atom in the presence of an electric field, in semi-parabolic coordinates $\dot{u}-u$, $n = 27$, $l = 1$. The plot on the left is for $F = 0.3$ au and the plot on the right is for $F = 0.45$ au.

Appendix A: Equations of motion for an electron in the Stark system

Here we present a detailed description of the equations of motion obtained for the Lagrangian and the numerical methods used to solve them.

The Lagrangian for a particle is given by

$$L = T - U$$

where $T$ is the kinetic energy and $U$ the potential energy of the particle. The kinetic energy for an electron in atomic units [6] is given by

$$T = \frac{1}{2}(\dot{x}^2 + \dot{y}^2 + \dot{z}^2)$$

Therefore, for an electron in the Na Rydberg state, the Lagrangian is given by

$$\frac{1}{2}(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) + \frac{1}{r} + \frac{(Z - 1)e^{-\alpha r}}{r} - F_z$$
where \( r = \sqrt{x^2 + y^2 + z^2} \). Therefore, using Lagrange’s equation of motion (1), we get

\[
\ddot{x} = - \frac{[1 + (Z - 1)e^{-\alpha r}]x - \alpha x(Z - 1)e^{-\alpha r}}{r^3}
\]

\[
\ddot{y} = - \frac{[1 + (Z - 1)e^{-\alpha r}]y - \alpha y(Z - 1)e^{-\alpha r}}{r^3}
\]

\[
\ddot{z} = - \frac{[1 + (Z - 1)e^{-\alpha r}]z - \alpha z(Z - 1)e^{-\alpha r}}{r^3} + F
\]

Since no analytic solution to the above exists, a fourth-order Runge-Kutta numerical integrator [9] was used to compute the resulting orbit.

Since a chaotic orbit is extremely sensitive to initial conditions, the Dec VAX/VMS Alpha system was used to perform the calculations in a 64 bit environment. The resulting accuracy in each integration step was of the order of 1 part in \( 10^8 \). This meant that when the orbit of an electron (\( n = 10, \ l = 1 \)) in the hydrogen Rydberg atom was allowed to evolve in time, all points of the orbit were on a single ellipse after 10000 time periods.

**Appendix B: Computation of initial conditions for numerical integration of the equations of motion**

This section gives a brief description of the initialization procedure in the program used to solve the equations of motion mentioned in the Appendix A.
Figure 15: Phase Space Plots for the Na Rydberg atom in the presence of an electric field, in semi-parabolic coordinates \( \dot{u} - u \), \( n = 27 \), \( l = 1 \). The plot on the left is for \( F = 0.521075 \) au and the plot on the right is for \( F = 0.521085 \) au. Note the sensitive dependence on the field strength, which strongly suggests chaos.

To compute the orbit for a given system, the program takes as input the following parameters:

1. Form of the Core Potential (specified by \( 1/r \) or \( 1/r + (Z - 1)e^{-\alpha r}/r \))
2. Principle quantum number \( n \)
3. Azimuthal quantum number \( l \)
4. Direction of angular momentum vector \( \mathbf{L} \)
5. Direction of Runge-Lenz vector \( \mathbf{A} \)
6. Magnitude of electric field \( F \)

The program then computes the initial position and velocity for the electron from the above parameters. It is assumed that the electron starts from the pericenter of an elliptical orbit, whose
Figure 16: Bifurcation Diagram for the Na Rydberg atom, in the cartesian z coordinate, n = 27, l = 1. Perturbation in the orbit at F ≈ 0.521080 strongly suggests chaotic behaviour in that region. We look at the z coordinate at 20 different time sections as the field strength is increased. In the absence of an electric field, the orbit remains in the x-y plane (z = 0), and hence the z coordinate is the best variable to plot in the bifurcation diagram.

Lenz vector is given by A. Therefore, the initial position lies in the direction of the Lenz vector, at a distance $\sqrt{1 - l(l+1)/n^2}$ (pericenter) from the origin. At the pericenter, the velocity of the electron is tangent to the orbit, so that $|L| = |p||r|$, where r is the displacement vector. Then, given the magnitudes of $L (= \sqrt{l(l+1)})$ and $r (= \sqrt{1 - l(l+1)/n^2})$, the magnitude of $p$ is computed. Finally, since the velocity vector lies perpendicular to both L and A, its orientation is found using simple geometric methods. Knowing the magnitude and direction of $p$, the initial velocity of the electron is then computed.

A detailed description of the program is given in the technical manual written by the programmer.


