The diamagnetic Kepler problem in a semiconductor environment

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The Diamagnetic Kepler Problem in a Semiconductor Environment

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Declaration

I, Colin Bleasdale, declare that this thesis submitted in partial fulfilment of the requirements for the conferral of the degree Doctor of Philosophy, from the University of Wollongong, is wholly my own work unless otherwise referenced or acknowledged. This document has not been submitted for qualifications at any other academic institution.

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December 13, 2016
Abstract

This thesis focuses on the classically chaotic motion of a Rydberg electron in an external magnetic field, known as the diamagnetic Kepler problem. This area has been studied extensively in atomic systems since the first experimental observation of oscillations in atomic spectra in 1969 by Garton and Tomkins. In subsequent investigations, both theoretical and experimental, these oscillations were linked the closed classical orbits of Rydberg electrons excited at energies close to the ionization threshold. Under these excitation conditions, the electron goes into an spherically-symmetric, near-zero energy radially outgoing Coulomb wave, sections of which are turned back towards the nucleus by the external magnetic field, thereby causing interference between the outgoing and returning waves resulting in the oscillations observed in the experimental atomic spectra. This can be efficiently modelled using classical mechanics by considering small sections of the electron wave as classical electrons where the length of time taken for the classical electron to traverse a closed orbit back to the nucleus is related to the experimental oscillation period. Due to its relative simplicity, hydrogen was predominately chosen to investigate this phenomenon. However, the recent detection of associated effects in the n-type hydrogenic doping centres of silicon have provided a new testing ground for these effects. In the course of the work presented here, we discuss how the semiconductor environment provides new classical effects not available in atomic systems. We investigate the effects associated with anisotropy leading to the so-called anisotropic diamagnetic Kepler problem, and also what effect the position of the oscillations in the spectrum have on the underlying classical mechanics. We then explore effects related to the addition of an external electric field in the special-case geometries of parallel and perpendicular to the external magnetic field. A new simplified theoretical framework for the general case of arbitrary external-field geometry is also developed.
List of publications

The content of this thesis contains work which has been published in a number of peer-reviewed journal articles:

Journal articles


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Chapter 1

Introduction

The work presented in the following chapters focusses on the diamagnetic Kepler problem, which has been widely studied over many decades and is an important system to investigate the manifestation of classical chaos in quantised systems. The first experimental observation of this effect was made by Garton and Tomkins in 1969 [1] in which they observed oscillations in the spectrum of barium atoms in an external magnetic field at excitation energies around the ionisation energy. They noted that these oscillations occurred at a frequency of approximately 1.5 times the cyclotron period. An example of such oscillations are shown in Fig. 1.1(a) which were subsequently referred to as “quasi-Landau oscillations” and were the source of much interest over the following decades.

In subsequent investigations, it was found that quasi-Landau oscillations were linked to the chaotic motion of a hydrogenic electron in the plane perpendicular to the applied magnetic field [3]. This motion of the electron is generally referred to as the Garton-Tomkins (GT) orbit which is shown in Fig. 1.1(b) and (c). As experimental methods continued to improve, allowing higher resolution atomic spectra to be measured, the oscillations in the spectrum became more complex. At sufficiently high resolution, the oscillations disappear altogether as the resolution neared that required to resolve individual energy levels. More complex oscillation patterns suggested that orbits other than the GT orbit were contributing to the quasi-Landau oscillations. This was first found to be the case by Holle et al. [4] where they reported the experimental observation of a spectral oscillation at 0.64 times the cyclotron frequency. By taking the Fourier transform of the experimental spectra, the period of those oscillations is extracted which they were then able to match to an electron orbit outside of the perpendicular plane. Higher resolution experiments soon followed with Main et al. [5] reporting the observance of oscillations which were matched to a series of orbits related to the orbit found by Holle et al. [4] with increasing number of traversals of the magnetic-field axis. These are shown in Fig. 1.2.
Figure 1.1: (a) Absorption spectrum of barium atoms in an external magnetic field for energies close to the ionisation threshold. The data was taken from Ref. [1] with arrows added by Du et al. [2] showing the classically regular region on the right where energy levels are split by the diamagnetic term, and the chaotic region on the left where quasi-Landau oscillations occur with a frequency of \( \sim 1.5 \) times the cyclotron frequency. Panels (b) and (c) show \( \rho - z \) and \( x - y \) projections of the orbit identified as the GT orbit which is the source of the oscillations in panel (a). The orbit evolves with time along the arrows shown with the shading moving from red at launch to blue on return to the nucleus. Note that the red section of panel (b) is covered due to the exact overlap of the outgoing and returning path of the electron.

The diamagnetic Kepler problem at energies approaching the ionisation energy is known to be a classically chaotic system. Therefore, orbits with small variations in initial launch angle lose connection with each other over long periods of time as illustrated in Fig.1.3. However, over short time periods, order does exist and adjacent orbits form "bundles" where the relationship between adjacent trajectories is more or less preserved. This can also be seen in Fig.1.3 as the adjacent orbits remain closely linked for the trajectory paths shaded from red to green as they return towards the nucleus. As the number of trajectories in a bundle increases, so
Figure 1.2: The closed orbits identified by (1) Holle et al. [4] and (2)–(6) Main et al. [5] which were found to contribute to higher resolution atomic spectra quasi-Landau oscillations. The orbits found by Main et al. [5] are in fact an infinite series of orbits with increasing number of magnetic-field axis crossings, only the first 6 are shown here.

The physical mechanism by which these classical closed orbits produce quasi-Landau oscillations in atomic spectra is due to the wave-like nature of the orbiting electron. When the electron is optically excited to energies near the ionisation threshold, it goes into a near-zero-energy outgoing Coulomb wave which propagates with spherical-symmetry radially outwards. As this wave front moves further away from the nucleus, small sections of the wave front “packets” can be considered to follow classical mechanics. Some of these packets may be turned back towards the nucleus by the external magnetic field along orbits such as those presented in Figs. 1.1 and 1.2, and, as the returning wave approaches the nucleus, it interferes with the
outgoing wave, causing the quasi-Landau oscillations observed in atomic spectra. The papers of Du and Delos [2, 7, 8] provide a thorough and detailed treatment of every section of this problem, from the quantum region close to the nucleus, to utilising semiclassical mechanics to describe the electron wave packet as it follows classically chaotic trajectories, before returning to the quantum region close to the nucleus and interfering with the outgoing wave. This comprehensive approach provides much more detail and extracts much more information on the problem than utilising a classical model, such as the relative strengths of oscillations from different orbits. However, classical mechanics can provide the periods of closed orbits, allowing the recurrence peak positions in the Fourier transformed experimental spectra to be matched with classical closed trajectories at far less computational expense. As such, only the classical model for analysing closed trajectories is examined over the course of the work presented in the following chapters.

The majority of work in the literature on the diamagnetic Kepler problem has fo-
cussed around the simplest system to study theoretically, the hydrogen atom [2, 4–15]. The work of Holle et al. [4] and Main et al. [5], as mentioned above, focussed on high resolution measurements of atomic hydrogen spectra. In a later paper, Holle et al. [6] designed an experimental method by which the photon excitation energy and magnetic field were constantly adjusted in order to keep the underlying classical dynamics constant over the entire spectra. This “Constant Scaled Energy Spectroscopy” allowed the experimental identification of a wide variety of closed classical orbits and was a method adopted by many experimentalists in subsequent investigations. Wintgen et al. [9] and Schweizer et al. [11] provide a stability analysis of certain classical periodic orbits of the system and describe how closed classical orbits are born out of either the GT orbit, or an orbit parallel to the magnetic field, as the scaled energy is increased towards the ionisation energy in which the classical system exhibits chaotic properties. Both Du et al. [2] and Wintgen et al. [10] provide detailed analysis of a large number of closed classical trajectories which, in majority, have been identified in both calculated, and experimental spectra. De- lande et al. [14] provide a detailed analysis of the onset of chaos in both the classical and quantum features of the hydrogen atom as the magnetic-field strength becomes comparable to that of the Coulomb interaction. A comprehensive overview of the work on the hydrogen atom is presented by Friedrich et al. [13].

Whilst atomic hydrogen has been the main focus for work on the diamagnetic Kepler problem, measurements and calculations have been pursued for other atomic species such as barium [1, 16], sodium [17], and helium [18] in which the extra electron present in the system provides additional complications to the well understood hydrogen atom scenario. Due to the similarity between atomic orbitals and the envelope functions of donor states in isotropic semiconductors, we may expect the optical spectrum of $n$-doped semiconductors to also present quasi-Landau oscillations. To our knowledge, this has not yet been observed, however, relatively recently in 2009, quasi-Landau oscillations were observed by Chen et al. [19] in the anisotropic medium of phosphorus doped silicon. This opened a new pathway to observe the diamagnetic Kepler problem in a whole different environment and is the focus and inspiration behind much of the work presented in this thesis.

Chapter 2 begins the investigation by giving the basic classical theoretical framework around the diamagnetic Kepler problem along with some analysis which is pertinent to the measurements recently taken in the semiconductor environment of silicon [19]. A numerical investigation is then undertaken to explore the possibility of observation quasi-Landau oscillations in other widely utilised semiconductors. In Chap. 3, the theoretical framework is extended to include the effects of an anisotropic electron
mass such as occurs in silicon. A numerical investigation is then undertaken for the specific case of silicon to observe how the effects of anisotropy manifest themselves in the classical electron orbits. Chapter 4 then extends the isotropic theoretical framework developed in Chap. 2 to include the effect of applying an electric field in the same direction as the applied magnetic field. Interesting numerical results are then presented with a specific focus on effects which may be observable in the case of silicon. Chapter 5 then looks at the case of the electric field being applied perpendicular to the external magnetic field. In this case, the rotational symmetry of the system is broken and calculations become much more difficult. In this chapter, we present a new theoretical framework which extends the conventions adopted in Chaps. 2 and 4 for the case of arbitrarily aligned external fields. This allows the calculation of classical electron orbits in a more simplified manner than had been previously available. A numerical analysis is then presented, again with a specific focus on effects which may be observable in silicon.
Chapter 2

Diamagnetic Kepler problem

2.1 Introduction

In this chapter, we begin in Sec. 2.2 by establishing the classical theoretical framework for a hydrogenic electron in an external magnetic field and show that by scaling, and utilising semiparabolic coordinates, as is the convention for this problem [10], the equations of motion can be derived. Using this scaling method, the equations of motion are dependent only on the one parameter, the scaled energy, rather than the energy of the electron and magnetic-field strength separately. The use of semiparabolic coordinates eliminates the Coulomb singularity from the equations of motion. This is important as the diamagnetic Kepler problem deals with orbits which start and finish essentially at the nucleus. Sec. 2.3 then utilises the equations of motion defined in the previous Sec. 2.2 to calculate all the closed orbits of the system at the ionisation threshold. We then show that utilising a positive scaled energy value, we are able to provide a better fit to the data available for silicon [19]. The effect of increasing the scaled energy is then investigated for both the entire spectrum of closed orbits and the 10 most stable orbits as determined by Du et al. [2]. In Sec. 2.3.1, we investigate the possibility of observing quasi-Landau oscillations in 11 widely used semiconductors, and in the process, determine experimental limits to the doping concentration and magnetic field strength relevant to each specific material. The main results are then discussed in Sec. 2.4.

2.2 Theory

Assuming an isotropic electron mass, the equations of motion can be written in Cartesian coordinates \((x_j, j = 1, 2, 3)\) as

\[
m \ddot{x}_j = -\frac{e^2 x_j}{4\pi\varepsilon_0 r^3} - eB(\dot{r} \times \mathbf{u})_j, \tag{2.1}
\]
where $\mathbf{r}$ is the radial vector and $\mathbf{u} = \mathbf{B}/B$ is a vector whose components are the direction cosines of the magnetic field.

Wintgen et al. showed that the classical equations of motion are invariant when scaling the distance and time by $\tilde{r} = r/\lambda$ and $\tilde{t} = t/T_c$ respectively [10]. The equations of motion can now be written in the form

$$\frac{d^2 \tilde{x}_j}{d\tilde{t}^2} = -\frac{\tilde{x}_j}{r^3} - 2\pi \frac{d\tilde{r}}{d\tilde{t}} \times u_j,$$

where $T_c = 2\pi/\omega_c$ is the cyclotron period, $\omega_c = eB/m$ is the cyclotron frequency and

$$\lambda = \sqrt{\frac{\pi m}{eB^2}},$$

which, for Si in a magnetic field of 4 T, is approximately 77 nm.

By utilising a rotating reference frame at the Larmor frequency $\omega_c/2$, the Lorentz force no longer depends on the velocity of the particle [10]. To prove this, we begin by considering the cyclotron motion of an electron shown in Fig. 2.1, with the magnetic field oriented along the $z$-axis and travelling at constant velocity $v = \omega_c/2$. In this case, the Lorentz force acts radially inwards at constant magnitude $F_{Lor} = evB = e\omega_cB/2$, and is equal to the centripetal force $F_{Cen} = mv^2/R = m\omega_c^2/4R$ where $R$ is the radius of the electron, which and can be found to be $R = 1/2$ in scaled coordinates. The position of the electron in Fig. 2.1 can therefore be expressed in scaled coordinates as

$$\tilde{x}(\tilde{t}) = \frac{1}{2} \cos(\pi \tilde{t}),$$

$$\tilde{y}(\tilde{t}) = \frac{1}{2} \sin(\pi \tilde{t}),$$

and

$$\tilde{z}(\tilde{t}) = \text{constant}.$$

Therefore, the velocity of the electron may be expressed as

$$\frac{d\tilde{x}(\tilde{t})}{d\tilde{t}} = -\frac{\pi}{2} \sin(\pi \tilde{t}),$$

$$\frac{d\tilde{y}(\tilde{t})}{d\tilde{t}} = \frac{\pi}{2} \cos(\pi \tilde{t}),$$

and

$$\frac{d\tilde{z}(\tilde{t})}{d\tilde{t}} = 0.$$
CHAPTER 2. DIAMAGNETIC KEPLER PROBLEM

Figure 2.1: Cyclotron motion of the electron in the $x$-$y$ plane. The magnetic field is aligned along the $z$-axis with the electron travelling at a constant velocity $v = \omega_c/2$. Therefore, the Lorentz force equals the centripetal force which acts radially inward on the electron.

Equation 2.2 may now be expressed in terms of the rotating reference frame as

$$\frac{d^2 \dot{x}_j}{dt^2} = -\frac{\dot{x}_j}{\bar{r}^3} - \pi^2 (1 - \delta_{j,3}) \dot{x}_j,$$

(2.10)

where $\delta$ is the Kronecker delta.

Equation 2.10 is related to the classical energy by

$$\mathcal{E}_c = \sum_{j=1}^{3} \frac{\dot{x}_j^2}{2} - \frac{1}{\bar{r}} + \frac{\pi^2}{2} \left[ \dot{x}_1^2 + \dot{x}_2^2 \right].$$

(2.11)
In scaled cylindrical coordinates ($\tilde{\rho}, \tilde{\phi}, \tilde{z}$), Eq. 2.11 can be written as

$$E_c = \frac{\dot{\tilde{\rho}}^2}{2} + \frac{(L_3)^2}{2\tilde{\rho}^2} + \frac{\dot{\tilde{z}}^2}{2} - \frac{1}{\tilde{\rho}} + \frac{\pi^2}{2} \tilde{\rho}^2,$$

(2.12)

where $L_3 = \tilde{\rho} \dot{\tilde{\phi}}$. We take the case of $L_3 = 0$ and introduce semiparabolic coordinates which allow the removal of the Coulomb singularity at the nucleus. In terms of semiparabolic coordinates $u$ and $v$, the cylindrical coordinates are

$$\tilde{\rho} = uv,$$  

(2.13)

$$\tilde{z} = \frac{1}{2}(u^2 - v^2),$$  

(2.14)

and the spherical coordinate $r$ is

$$\tilde{r} = \frac{1}{2}(u^2 + v^2).$$  

(2.15)

By introducing a scaled time

$$\frac{dt}{d\tau} = \tilde{r},$$  

(2.16)

the velocities in semiparabolic coordinates can be expressed as

$$\dot{\tilde{\rho}} = \frac{2(v\dot{u} + u\dot{v})}{u^2 + v^2},$$  

(2.17)

and

$$\dot{\tilde{z}} = \frac{2(u\dot{u} - v\dot{v})}{u^2 + v^2},$$  

(2.18)

where dots denote differentiation with respect to the scaled time $\tau$. Equation 2.12 can now be simplified to

$$\frac{(\dot{u}^2 + \dot{v}^2)}{2} - \frac{E_c(u^2 + v^2)}{4} + \frac{\pi^2 u^2 v^2 (u^2 + v^2)}{8} = \frac{1}{2}. $$

(2.19)

With the Coulomb singularity avoided through the use of semiparabolic coordinates, the equations of motion can be found from Eq. 2.19 using Hamilton’s equations, and are given by

$$\ddot{u} = -\pi^2 \left[ \frac{u^3 v^2}{2} + \frac{uv^4}{4} \right] + \frac{E_c u}{2},$$

(2.20)

and

$$\ddot{v} = -\pi^2 \left[ \frac{u^2 v^3}{2} + \frac{u^4 v}{4} \right] + \frac{E_c v}{2}.$$

(2.21)
CHAPTER 2. DIAMAGNETIC KEPLER PROBLEM 11

The energy $\mathcal{E}_c$ is scaled as

$$\mathcal{E}_c = \mathcal{E}_q \gamma^{-2/3} \left( \frac{\pi^2}{2} \right)^{1/3},$$

(2.22)

where $\mathcal{E}_q$ is the quantum mechanical energy counterpart to the classical energy $\mathcal{E}_c$ (measured in Rydbergs) and $\gamma$ is the dimensionless measure of the magnetic field given by

$$\gamma = \frac{\hbar e B}{2R_y^* m},$$

(2.23)

where $R_y^* = e^4 m/(32\pi^2\epsilon^2\hbar^2)$ is the effective Rydberg and $\epsilon = \epsilon_0\epsilon_r$ is the absolute value of the static dielectric permittivity.

Electrons are launched from the nucleus in semiparabolic coordinates using Eqs. 2.20 and 2.21 at angles from 0–180$^\circ$ from the $x$-$z$ plane with the magnetic field aligned along the $z$-axis. Due to the symmetry of the isotropic case, an angular launch range of 0–90$^\circ$ would be sufficient to identify unique closed orbits of the system. However, we use the larger range above to make comparisons with work in later chapters more straightforward. Trajectories for which the electron returned to within 0.001$\lambda$ of the nucleus where considered as closed orbits. As the system is chaotic, order is only maintained between adjacent orbits for a short period of time [2], therefore we restrict the important orbits of the system to those returning within 5$T_c$.

### 2.3 Numerical results

We begin our numerical analysis by reproducing some basic results from the literature. Du et al. [2] provide a list of the 65 most important orbits of the system which return to the nucleus in less than 10$T_c$ at a scaled electron energy of $\mathcal{E}_c = 0$, corresponding to the ionisation energy of the electron. We do not intend to reproduce all 65 of those orbits here. However, to show the theoretical framework outlined in Sec. 2.2 is valid, Fig. 2.2 shows the first 10 orbits in Fig. 8 of Ref. [2] along with their associated launch angles and periods.

We can see from Fig. 2.2, that we are able to reproduce the same orbit shapes as those seen in Fig. 8 of Ref. [2] with identical launch angles. However, our periods are slightly different. This is due to the fact that we are launching directly from the nucleus, whereas in Ref. [2], they launched from a small finite distance. Therefore, our periods are slightly longer than those presented in that publication.

Next, we calculated the entire spectrum of closed orbits at $\mathcal{E}_c = 0$ for a constant
Figure 2.2: Orbits 1–10 as labelled in Fig. 8 of Ref. [2]. The magnetic field is oriented along the $z$ axis. The classical energy of the electron is $E_c = 0$, placing it right at the ionisation threshold. The shading of the orbit path evolves with time as the orbit describes a closed path along the arrows drawn. Orbits are labelled by the lead author of the publication “Du” followed by the number of the orbit. Labels within the orbit plots denote the launch angle “$\theta$” and the period of the orbit “$T/T_c$”. These conventions will all be adopted for the duration of this work.
Figure 2.3: The return distance ($r_{ret}$) to the nucleus as a function of polar launch angle for (a) the entire angular spectrum and (b) angles close to the GT orbit at $90^\circ$. The electron energy is still $E_c = 0$ and only orbits who return within $0.001\lambda$ of the nucleus in less than $5T_c$ are shown. Data points are shaded according to their orbital period in the range of $0 - 5T_c$ as indicated by the bar at the bottom of the figure. This convention will be adopted for the duration of this work.

We define a closed orbit as any trajectory which returns within $0.001\lambda$ of the nucleus within $5T_c$. The choice of $0.001\lambda$ as our return distance cutoff is to ensure that the electron returns to a distance less than the Bohr radius to the nucleus. Displayed in Fig. 2.3 (a) are the results for the electron return distance ($r_{ret}$) to the nucleus as a function of polar launch angle. Using this representation, we are able to gain a clear overall picture of the entire system. The chaotic nature of system is visible as slight variations in launch angle lead to large changes in the return distance to the nucleus. If we zoom in on a small angular section, such as in Fig. 2.3 (b) around the GT orbit, we can see that as the polar launch angle is varied, the return distance shows a parabolic dispersion due to the stable nature of this orbit. For successive harmonics of the GT orbit, this dispersion parabola increases in curvature as the longer period of the orbit decreases its relative stability. We can also see just how stable this orbit is compared to other closed orbits surrounding it at $87.5$ and $92.5^\circ$ in which only relatively few adjoining orbits meet the criteria of a closed orbit. We refer to these parabolic dispersions of adjacent orbits as bundles, and denote the number of orbits in each bundle as $N_{bun}$. This parameter gives an indication of the relative stability of different orbits.

We now turn our attention to the semiconductor environment, specifically silicon in which this phenomenon was recently observed within such a system for the first time [19]. Whilst we believe the experimental results presented in this publication to be very good, there were some faults we have identified with the theoretical analysis.
The first being that the anisotropy of silicon was not fully explored. This will be addressed later in Chap. 3. The second was that the cyclotron frequency was incorrectly calculated, and thirdly, they utilised a scaled electron energy of \( E_c = 0 \). This is quite a common scaled energy used in the analysis of atomic spectra, however, in the spectra presented in Ref. [19], the oscillations are present at energies well above the ionisation threshold. We estimate the oscillations occur over a scaled-energy range of \( 0 \leq E_c \leq 8.8 \). By coincidence, the second and third problems described above act to cancel each other, and some agreement between theory and experiment is achieved in Ref. [19]. An illustration of just how much the system changes over a section of this scaled-energy range is given in Fig. 2.4.

We can see that as the energy is increased to approximately the midpoint of the oscillation range given in the previous paragraph, not only are there far fewer closed orbits, but they exist over a much narrower range of polar launch angles. The consequence of this constriction of allowed polar launch angles becomes more obvious if the orbit periods are explicitly observed as in Fig. 2.5. In this representation, we can see that the orbit periods have congregated together into groups which roughly represent increasing harmonics of the GT orbit. This is due to the orbits being more constrained to launch angles close to the plane perpendicular to the magnetic field. It is also quite apparent from Fig. 2.5 that utilising a scaled energy of \( E_c = 4 \) provides a close match between theory and experiment, especially for the first, third, and fifth experimental peaks. However, due to the large energy range over which these oscillations exist in the experimental spectra shown in Ref. [19], the method of making a simple Fourier transform over the oscillation range to extract the oscillation periods is not entirely accurate due to the large change in the system over this energy range [7]. Therefore, the peak positions shown here are to be taken as estimates.

To illustrate the change in orbit behaviour as the scaled field is raised to \( E_c = 4 \), Figs. 2.6–2.14 show the evolution of the orbits depicted in Fig. 2.2 as the scaled energy is increased from \( E_c = 0 – 4 \) in integer steps. Clearly, the orbits which are still observable, have been compressed closer to the perpendicular plane as is shown by their respective polar launch angles. There is also a large increase in the individual orbit periods which is to expected at a higher scaled energy, and, is the predominant reason for the simple Fourier transform no longer being applicable to analyse the experimental data. At \( E_c = 4 \), the orbits denoted as “Du6” and “Du7” become indistinguishable from the orbits denoted as “Du1” and “Du2” respectively as their polar launch angles practically coincide at these high energies. Orbit “Du9” has been omitted in this investigation as its period exceeds \( 5T_c \). Table 2.1 details
Figure 2.4: The return distance ($r_{\text{ret}}$) to the nucleus as a function of polar launch angle as the scaled energy is varied over the range $\mathcal{E}_c = 0 - 4$ in integer steps.
**CHAPTER 2. DIAMAGNETIC KEPLER PROBLEM**

**Figure 2.5:** The return distance \( (r_{\text{ret}}) \) to the nucleus as a function of orbit period for (a) \( E_c = 0 \) and (b) \( E_c = 4 \). Thick red lines represent the experimental peak positions shown in Fig. 3(a) of Ref. [19] with approximate positions of \( T/T_c \approx 0.87, 2.04, 2.78, 3.35, \) and 4.66. Data points are uncoloured here due to the orbit periods being explicitly shown.

The launch angle \( \theta \), orbit period \( T \), return distance to the nucleus \( r_{\text{ret}} \), maximum distance from the nucleus \( r_{\max} \), and the number of orbits in each bundle \( N_{\text{bun}} \) for all of the orbits given in Figs. 2.6–2.14. Table 2.1, in addition to displaying all of the information detailing how the orbits are compressed into the perpendicular plane, the relative stability of the orbits is greatly impacted by the increasing scaled energy. Not only for individual orbits of different energies, but also between the orbits themselves. For example, at \( E_c = 1 \), “Du4” is more stable than “Du5”, however, at \( E_c = 2 \), “Du5” is now more stable than “Du4”.

**Figure 2.6:** Orbit “Du1” as labelled in Fig. 2.2(a) (the GT orbit). The classical energy of the electron is varied from \( E_c = 0 – 4 \) in integer steps, which, at \( E_c = 4 \), places it right at the midpoint of the oscillations seen in Ref. [19].
CHAPTER 2. DIAMAGNETIC KEPLER PROBLEM

Figure 2.7: As for Fig. 2.6, but for the orbit denoted as “Du2”. 

Figure 2.8: As for Fig. 2.6, but for the orbit denoted as “Du3”. 

Figure 2.9: As for Fig. 2.6, but for the orbit denoted as “Du4”. 

Figure 2.10: As for Fig. 2.6, but for the orbit denoted as “Du5”. 

\[ \frac{z}{\Lambda} \] 

\[ \frac{\theta}{\Lambda} \] 

\[ \frac{T}{T_c} \] 

\[ \rho/\Lambda \] 

\[ c \]
<table>
<thead>
<tr>
<th>Orbit index</th>
<th>$\mathcal{E}_c$</th>
<th>$\theta$ (degrees)</th>
<th>$T/T_c$</th>
<th>$r_{ret}/\lambda$</th>
<th>$r_{max}/\lambda$</th>
<th>$N_{bun}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>90</td>
<td>0.666667</td>
<td>1.23 $\times 10^{-8}$</td>
<td>0.587368</td>
<td>2663</td>
<td></td>
</tr>
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</tr>
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<td>Du1</td>
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<td></td>
</tr>
<tr>
<td>3</td>
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<td>4.72 $\times 10^{-8}$</td>
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<td>783</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>90</td>
<td>0.866035</td>
<td>1.71 $\times 10^{-9}$</td>
<td>1.00598</td>
<td>613</td>
<td></td>
</tr>
<tr>
<td>Du2</td>
<td>2</td>
<td>71.439</td>
<td>1.71812</td>
<td>5.80 $\times 10^{-9}$</td>
<td>0.859811</td>
<td>286</td>
</tr>
<tr>
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<td>0.94842</td>
<td>213</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>77.798</td>
<td>1.80397</td>
<td>2.10 $\times 10^{-7}$</td>
<td>1.0352</td>
<td>167</td>
<td></td>
</tr>
<tr>
<td>Du3</td>
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<td>2.71028</td>
<td>8.13 $\times 10^{-8}$</td>
<td>1.18635</td>
<td>121</td>
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<td>Du4</td>
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<td>75.504</td>
<td>2.54318</td>
<td>1.98 $\times 10^{-7}$</td>
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<td>64</td>
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<tr>
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<td>0.933923</td>
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<td>4</td>
<td>80.317</td>
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<td>2.24 $\times 10^{-7}$</td>
<td>1.02413</td>
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<td></td>
</tr>
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<td>Du5</td>
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<td>61.357</td>
<td>3.71315</td>
<td>7.02 $\times 10^{-8}$</td>
<td>1.37672</td>
<td>67</td>
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<tr>
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<td>66.694</td>
<td>3.75458</td>
<td>3.38 $\times 10^{-8}$</td>
<td>1.41238</td>
<td>51</td>
<td></td>
</tr>
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<td>70.323</td>
<td>3.78696</td>
<td>3.99 $\times 10^{-7}$</td>
<td>1.45241</td>
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<td>Du6</td>
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<td>89.104</td>
<td>2.54318</td>
<td>1.98 $\times 10^{-7}$</td>
<td>0.83923</td>
<td>64</td>
</tr>
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<td>89.559</td>
<td>2.60947</td>
<td>9.43 $\times 10^{-6}$</td>
<td>0.953394</td>
<td>12</td>
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</tr>
<tr>
<td>4</td>
<td>90</td>
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<td>2.24 $\times 10^{-7}$</td>
<td>1.02413</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>Du7</td>
<td>2</td>
<td>71.199</td>
<td>2.52711</td>
<td>6.78 $\times 10^{-7}$</td>
<td>0.869643</td>
<td>14</td>
</tr>
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<td>2.60947</td>
<td>3.23 $\times 10^{-7}$</td>
<td>0.953334</td>
<td>7</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>77.798</td>
<td>2.70113</td>
<td>2.24 $\times 10^{-7}$</td>
<td>1.02413</td>
<td>-</td>
<td></td>
</tr>
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<td>Du8</td>
<td>2</td>
<td>59.343</td>
<td>4.71709</td>
<td>1.83 $\times 10^{-8}$</td>
<td>1.65666</td>
<td>43</td>
</tr>
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<td>64.924</td>
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<td>9.37 $\times 10^{-7}$</td>
<td>1.68145</td>
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<td>4</td>
<td>68.727</td>
<td>4.78792</td>
<td>1.20 $\times 10^{-7}$</td>
<td>1.70957</td>
<td>27</td>
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<td>Du10</td>
<td>2</td>
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<td>3.51264</td>
<td>5.05 $\times 10^{-7}$</td>
<td>1.10342</td>
<td>24</td>
</tr>
<tr>
<td>3</td>
<td>79.485</td>
<td>3.60836</td>
<td>5.84 $\times 10^{-7}$</td>
<td>1.16469</td>
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<td>4</td>
<td>81.217</td>
<td>3.67447</td>
<td>4.90 $\times 10^{-6}$</td>
<td>1.22608</td>
<td>14</td>
<td></td>
</tr>
</tbody>
</table>

Table 2.1: The polar launch angle $\theta$, the period $T/T_c$, the return and maximum distances, and the bundle number $N_{bun}$, for different values of the classical energy $\mathcal{E}_c$ for orbits “Du1” – “Du10”, excluding “Du9” as it has a period greater than $5T_c$. Orbits are indexed according to the convention outlined in Fig. 2.2.
Figure 2.11: As for Fig. 2.6, but for the orbit denoted as “Du6”. This orbit becomes unstable between $\mathcal{E}_c = 3 - 4$ due to the launch angle coinciding with the GT orbit in Fig. 2.6 (e).

Figure 2.12: As for Fig. 2.6, but for the orbit denoted as “Du7”. This orbit becomes unstable between $\mathcal{E}_c = 3 - 4$ due to the launch angle coinciding with “Du2” at high energies in Fig. 2.7.

Figure 2.13: As for Fig. 2.6, but for the orbit denoted as “Du8”.

Figure 2.14: As for Fig. 2.6, but for the orbit denoted as “Du10”.

CHAPTER 2. DIAMAGNETIC KEPLER PROBLEM
2.3.1 Semiconductor candidates to observe diamagnetic Kepler problem

In this section, we look to explore the possibility of observing quasi-Landau oscillations in 11 widely utilised semiconductor materials. Given the recent observation of these oscillations in silicon [19], we look to provide answers to some of the questions these results have raised. Firstly, ‘Why had this not been observed previously?’ as spectra of semiconductor materials have been measured extensively for decades. Secondly, ‘Is silicon the best candidate to observe the diamagnetic Kepler problem in a semiconductor environment?’ as isotropic materials such as gallium arsenide may provide a simplified comparison between available theory and experiment. Lastly, ‘Are there improvements that can be made experimentally, or in the analysis of data, to observe the interference from classical electron trajectories?’ In this section, we aim to answer questions one and two by providing the experimental conditions needed to observe quasi-Landau oscillations across a range of widely utilised semiconductors. The final question will be discussed with reference to experimental and analytical techniques employed in atomic measurements or the diamagnetic Kepler problem.

The theoretical model we use to analyse all semiconductor candidates is described earlier in Sec. 2.2. As this model is only valid for an isotropic electron mass, we will use an isotropic approximation for all of the semiconductors discussed. While this is an excellent approximation for some of the materials (gallium arsenide) others, such as silicon, are distinctly anisotropic. However, as anisotropy itself is neither a determining factor for the observation of these orbits, nor does it distort the results substantially enough to render the use of an isotropic approximation as unacceptably inaccurate, anisotropy will be neglected in the following investigation.

The materials we are investigating in this work are shown in Tab. 2.2, along with the physical parameters important for this work [20]. The maximum field corresponds to the condition that \( \lambda \geq 10a^* \) where \( a^* \) is the effective Bohr radius and ensures orbits travel sufficiently far from the impurity.

In order for the impurity centres to be considered as isolated, we assume the impurities constitute a simple cubic lattice of \( 20\lambda \) as the important electron orbits are confined within a few \( \lambda \) of the impurity centre. Given this condition, and the parameters given in Tab. 2.2, we can find the upper bound to the impurity concentration as a function of magnetic field. This is shown in Fig. 2.15.
<table>
<thead>
<tr>
<th>Semiconductor</th>
<th>Mass ((m_0))</th>
<th>(\varepsilon_r)</th>
<th>Maximum Field (T)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Silicon (Si)</td>
<td>0.26</td>
<td>11.4</td>
<td>24.2</td>
</tr>
<tr>
<td>Germanium (Ge)</td>
<td>0.12</td>
<td>16</td>
<td>2.62</td>
</tr>
<tr>
<td>Aluminium Nitride (AlN)</td>
<td>0.4</td>
<td>8.5</td>
<td>103</td>
</tr>
<tr>
<td>Gallium Nitride (GaN)</td>
<td>0.2</td>
<td>8.9</td>
<td>23.5</td>
</tr>
<tr>
<td>Gallium Phosphide (GaP)</td>
<td>0.35</td>
<td>11.1</td>
<td>46.2</td>
</tr>
<tr>
<td>Gallium Arsenide (GaAs)</td>
<td>0.063</td>
<td>13.1</td>
<td>1.08</td>
</tr>
<tr>
<td>Gallium Antimonide (GaSb)</td>
<td>0.041</td>
<td>15.7</td>
<td>0.317</td>
</tr>
<tr>
<td>Indium Nitride (InN)</td>
<td>0.11</td>
<td>15.3</td>
<td>2.40</td>
</tr>
<tr>
<td>Indium Phosphide (InP)</td>
<td>0.08</td>
<td>12.5</td>
<td>1.91</td>
</tr>
<tr>
<td>Indium Arsenide (InAs)</td>
<td>0.023</td>
<td>15.15</td>
<td>0.107</td>
</tr>
<tr>
<td>Indium Antimonide (InSb)</td>
<td>0.014</td>
<td>16.8</td>
<td>0.0323</td>
</tr>
</tbody>
</table>

Table 2.2: List of semiconductors analysed in this section along with their important physical parameters. Here \(m_0\) is the free electron mass and \(\varepsilon_r\) is the relative permittivity of the semiconductor. The maximum fields for each material are also listed as shown in Fig. 2.15. For materials which are generally considered anisotropic, the effective mass of the electron is taken as the effective conductivity mass \([20]\). This is calculated using the harmonic mean of the effective masses along the three crystallographic directions.

**Figure 2.15:** Upper bound for impurity concentration in various semiconductors as a function of magnetic field in order for electron orbit isolation to be satisfied. Each line is cut off at that material’s associated maximum magnetic field as given in Table 2.2. The order of appearance of curves from left to right is InSb, InAs, GaSb, GaAs, InP, InN, Ge, GaN, Si, GaP and AlN. The legend order of appearance is from smallest atomic weight at the top to greatest at the bottom.
Figure 2.15 shows that, compared to many of the other semiconductors, silicon is required to be one of the most pure crystals in order for this effect to be observed at low fields, with indium antimonide and indium arsenide having the least stringent dependence on purity. On the other hand, due to their associated maximum fields, these materials are not suitable to the observation of electron orbits. From this rather straight forward analysis, it would seem that silicon is quite a good candidate along with gallium nitride, gallium phosphide and aluminium nitride due to their wide magnetic field ranges, and therefore, higher upper bounds for their associated doping concentrations. Materials such as germanium, indium nitride, indium phosphide and gallium arsenide may be suitable for study in low fields. However, this requires low doping concentrations. Achieving doping concentrations as low as $1 \times 10^8 \text{cm}^{-3}$ is problematical. At values this low, detection via optical methods may become difficult.

We will now look at how these conditions manifest themselves in the electron orbits and possible experimental results. Quantities such as the orbit periods and the classical energy of the electron relative to both the magnetic field and photon energies vary across materials. If we take the case of an applied field of 4T, which was considered in the experimental paper on silicon [19], we can compare the corresponding classical energies in each of these materials. Given this field is in some cases larger, or smaller, than the associated material’s maximum field, we may see how this condition manifests itself in the results. Firstly, in Fig.2.16, we consider a classical electron energy of $E_c = 4$, (which was shown to be an important value for silicon in Sec.2.3), and calculate the photon energy ($E_q$) this equates to at an applied field of 4T for various materials.

We can see from Fig.2.16 that while these parameters in silicon represent a photon energy of $51.6 \text{cm}^{-1}$ (the midpoint of the oscillations observed in Ref.[19]), in other materials this can be much larger, such as in indium antimonide and indium arsenide, whose classical energy of $E_c = 4$ places them around $100 \text{cm}^{-1}$ above the ionisation threshold. Therefore, using a classical energy of $E_c = 4$ in the comparison between different materials would only suffice if the oscillations occurred over varying spectral ranges for different materials.

We can also investigate how fixing the classical energy of $E_c = 4$ affects the orbit periods themselves. In Fig.2.17 we show the closed orbit periods at a field of 4T for different materials at a classical electron energy of $E_c = 4$. We can see that for materials with a maximum field less than 4T the orbit periods are squashed together. Resolving orbits under these conditions is almost impossible experimen-
Figure 2.16: Photon energy as a function of magnetic field with a classical electron energy of $E_c = 4$. The order of appearance of curves from top to bottom is InSb, InAs, GaSb, GaAs, InP, GaN, InN, AlN, Ge, Si and GaP. The legend order of appearance is from smallest atomic weight at the top to greatest at the bottom.

tally, given the peak widths in the data presented for silicon [19]. Reducing the magnetic-field strength to a field below this maximum will spread these orbit periods out and increase the chances to resolve them. However, in reducing the field, the peak strengths associated with closed orbits in the data weaken as is also seen in the data presented in silicon [19]. Therefore, materials which have a maximum field greater than 4 T provide the best medium for the observance of this effect under these conditions.

We will now assume that the spectral oscillations in these materials occur over the same spectral width as has been observed in silicon. Therefore, the midpoint value in silicon of 51.6 cm$^{-1}$ now remains fixed, and different values of the classical energies for each material will be needed in order for this condition to be satisfied. Figure 2.18 shows how the classical energies vary for these materials under this condition. We can see that in order for this condition to be met, the classical energy varies in the range $E_c = 2 - 4.5$ depending on the material.

Given different materials under this condition need to be considered with varying classical electron energies, the orbit periods will be different to those presented in Fig. 2.17. Figure 2.19 shows the orbit periods for these materials with the energies found in Fig. 2.18.
Figure 2.17: Orbit period comparisons with classical electron energy of $E_c = 4$ for different semiconductors at a magnetic field of 4T. As the classical electron energy is constant across all materials, these results are simply scaled to one another by the different cyclotron frequencies of each material.
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Figure 2.18: Classical energy of the electron as a function of magnetic field at a spectral position of 51.6 cm$^{-1}$, focusing on the region around 4 T. The order of appearance of curves from top to bottom is GaP, Si, Ge, AlN, InN, GaN, InP, GaAs, GaSb, InAs and InSb. The legend order of appearance is from smallest atomic weight at the top to greatest at the bottom.

The orbit periods in Fig. 2.19 look very similar to those in Fig. 2.17. This is due to the fact that in the materials whose orbit periods are relatively spread out (aluminium nitride, gallium nitride and gallium phosphide), the classical electron energies are quite close to $E_c = 4$ (3.72, 3.04 and 4.25 respectively). Therefore, the difference in orbit periods for these materials in relation to those presented in Fig. 2.17 is quite minor. The largest differences are in those materials whose orbits are more compressed, (indium antimonide, indium arsenide and gallium antimonide); however, due to this compression, the differences in orbit periods are difficult to discern and do not improve the experimental resolution of the orbits in these materials. The effect of varying the classical energy is that as the classical energy is increased from $E_c = 0$, the orbits converge together into multiples of the GT period. This happens due to the reduction of angles over which closed orbits can be identified as was pointed out in Sec. 2.3. At a classical energy of $E_c = 0$, these orbits can be identified for polar launch angles up to approximately 65° above the $z = 0$ plane. However, at a classical energy of $E_c = 4$ this range decreases to approximately 25° above the $z = 0$ plane. Therefore the orbits are being compressed to resemble harmonics of the GT period as the classical energy is increased.

In addition to the preceding numerical results, we return to the final question posed at the beginning of this section and suggest that the experimental method proposed by Holle et al. in Ref. [6], and subsequently utilised in Refs. [18, 21, 22], may im-
Figure 2.19: Orbit period comparisons with photon energy 51.6 cm\(^{-1}\) for different semiconductors at a magnetic field of 4 T. As the classical electron energy is now different in each material, Eq. 2.20 and 2.21 need to be solved in each case.
prove the resolution of these electron orbit periods. This is a method called Constant Scaled Energy Spectroscopy, which involves adjusting the magnetic field and incident frequency on the sample to hold $E_c$ constant. This will reduce the dispersion of the electron orbit peaks as the oscillations in the spectrum observed in silicon [19] occur over an energy range of approximately $E_c = 0 - 8.8$, which has a large effect on the observed electron periods of the system. Constant Scaled Energy Spectroscopy will also resolve an issue raised earlier where it was pointed out that the Fourier transform method of analysing the data could only be taken as an approximation due to the large classical energy range the oscillations in the spectrum covered. Alternatively, this problem in the Fourier transform can be addressed using the chirped Fourier transform method to analyse experimental data as outlined by Freund et al. [23]. Both this method of chirped Fourier transform and Constant Scaled Energy Spectroscopy should lead to sharper peaks of the electron orbit periods and may also lead to more orbits being identified than previously observed for silicon in Ref. [19].

2.4 Conclusion

In this chapter, we focussed on the diamagnetic Kepler problem, specifically, the classically chaotic motion of a hydrogenic electron in an external constant magnetic field. In Sec. 2.2, we developed the classical equations of motion for this hydrogenic electron utilising the well known scaling properties of the hydrogen atom, a reference frame rotating at $\omega_c / 2$, and semiparabolic coordinates to avoid the Coulomb singularity at the nucleus [10]. As a consequence, the equations of motion given in Eqs. 2.20 and 2.21 are only dependent upon the scaled energy $E_c$ rather than both the energy and magnetic-field separately. Given the diamagnetic Kepler problem is associated with the classically chaotic closed orbits of a hydrogenic electron, we define a closed orbit as returning within 0.001\(\lambda\) of the nucleus. This condition ensures that the electron returns to a distance less than the Bohr radius to the nucleus. We then limited our investigation to orbits returning to the nucleus in less than a scaled time of $5T_c$, as these are the most important orbits in analysing the available experimental data in silicon [19], and are generally the most stable orbits classically.

In Sec. 2.3, we first used the equations of motion derived in Sec. 2.2 to produce the ten most stable orbits as outlined in Fig. 8 of Ref. [2]. Having confirmed the equations of motion reproduce the results in the literature, the entire spectrum of orbits were calculated for the diamagnetic Kepler problem at the ionisation threshold ($E_c = 0$). However, in the semiconductor environment as we discuss in more detail in Sec. 2.3.1, the experimental results available show quasi-Landau oscillations in the spectrum, linked to closed classical orbits, extend to energies well in excess of
the ionisation energy [19]. Seemingly, this is a result not previously observed for experiments on atomic species, as the literature focusses predominantly on energies at, or below the ionisation threshold. We therefore proceeded to calculate the entire spectrum of orbits for positive integer values of the scaled energy up to $E_c = 4$, as this was found to be the midpoint of the oscillations observed in silicon [19]. We found that, as the scaled energy is increased, the spectrum of orbits compresses towards the perpendicular plane such that a narrower range of polar launch angles facilitate closed orbits. This is also reflected in the analysis of individual orbits. Using this scaled energy, we endeavoured to make a new comparison to the experiment in silicon, and found using a scaled energy of $E_c = 4$, rather than $E_c = 0$, gave a superior fit between experimental recurrence peak positions and closed orbit periods.

In Sec. 2.3.1, we investigated 11 different semiconductors as candidates for the experimental observation of the quasi-Landau resonances associated with the classically chaotic motion of electrons around impurity centres. The first result is that, regardless of which material is chosen, the sample is required to have a doping concentration no greater than $10^{12}$ cm$^{-3}$ for fields which can be reached in typical laboratories. This is quite a heavy constraint as samples are typically unintentionally doped to orders of magnitude above this limit. Such a low doping limit and low magnetic-field limit may provide an explanation for these oscillations not being observed previously in widely-used semiconductors such as gallium arsenide and germanium.

A second question addressed is whether silicon is the best candidate for the observation of this effect? While silicon is a better candidate than gallium arsenide or germanium, it was found that the lighter compounds such as aluminium nitride and gallium phosphide may provide a better medium for the detection of the effect. The orbits in these materials extend over a larger period range and therefore would be more easily resolvable in experiments, allowing for the possibility of more closed orbits being identified experimentally. Another way to improve resolution of recurrence peaks arising from classical electron orbits is to employ the method of Constant Scaled Energy Spectroscopy [6] or utilising a chirped Fourier transform [23] to analyse experimental data. Both of these techniques will provide sharper resolution of these peaks experimentally than has been achieved previously in silicon [19].
Chapter 3

Anisotropic diamagnetic Kepler problem

3.1 Introduction

The effect of anisotropy on chaotic systems involving classical orbits is not a new area of study. The anisotropic Kepler problem, the same system we study here but in absence of an external magnetic field, has been studied extensively as a quantum system whose classical counterpart exhibits chaotic properties. Contopoulos et al. [24] provide a detailed study on the value of anisotropic mass ratio and its impact on the underlying chaotic nature of the classical system. Work on this area is continuing to be pursued with Kubo et al. studying the statistical nature of the system [25] and the application of periodic orbit theory (as opposed to the closed orbit theory of the diamagnetic Kepler problem) to the classical orbits of the anisotropic Kepler problem [26].

Semiconductors have also played an important role to the study of chaotic systems and classical orbits. Fromhold et al. showed that oscillations in the current-voltage characteristics of gallium arsenide quantum well structures occur when an external magnetic field is applied at various orientations [27], and that these oscillations are linked to the unstable closed classical orbits of an electron within the confines of the quantum well [28]. Muller et al. analyse the angle of the magnetic field to the quantum well and the precursors of the system moving into a chaotic state [29]. Fromhold et al. also showed that chaos in semiconductor superlattices causes electron orbits to de-localize through stochastic webs leading to an increase in the electrical conductivity of the structure [30, 31].

In Chap. 2, various semiconductor materials were analysed for their potential suit-
ability to observe quasi-Landau oscillations stemming from closed classical electron orbits. In both Chap. 2, and Ref. [19], an average isotropic model for the pertinent valley of the conduction band, with the electron mass given by the cyclotron mass for each valley of the conduction band was utilised. Whilst this was sufficient for our purposes in Chap. 2, here we revisit the anisotropic medium of silicon in order to provide a detailed description of how an anisotropic electron mass effects the important closed classical electron orbits. In particular, we investigate the dependence of the duration and shapes of the closed orbits on the magnetic-field orientation and electron energy. We then make a new comparison to the available experimental results [19]. We begin with Sec. 3.2 which provides the theoretical framework for the inclusion of the effects of an anisotropic mass on the classical system. We show how the cyclotron motion of the electron, the energy scale, and the treatment of the Coulomb singularity are altered due to the presence of an anisotropic electron mass and set up the equations of motion for the classical system. In Sec. 3.3, we explore how the magnetic-field orientation effects the duration and shapes of closed classical orbits for the specific case of silicon, and in Sec. 3.4 we summarize the main results from the chapter.

3.2 Theory

In this section the main equations leading to the closed orbits are presented. Section 3.2.1 is devoted to solving the problem in the absence of the Coulomb interaction. This leads to the well-known expression for the cyclotron mass and establishes a natural time unit. Additionally, the shapes of the cyclotron orbits are described. In Sec. 3.2.2, the Coulomb interaction is included and dimensionless equations of motion are set up. In Sec. 3.2.3 an appropriate energy scale is introduced and its relation to the quantum mechanical approach is discussed, whereas Sec. 3.2.4 presents equations for the specific case of a valley in the conduction band of silicon. Finally, the treatment of the Coulomb singularity is given in Sec. 3.2.5.

3.2.1 Cyclotron Frequency

First we deal with the motion of an electron with anisotropic mass given by a diagonal matrix $1/m$ subject to a uniform magnetic field $B$. Since $(1/m)_{jj'} = m_j^{-1} \delta_{jj'}$, the components of the acceleration are given by

$$m_j \ddot{x}_j = -e (\dot{r} \times B)_j .$$

(3.1)
Hence, the acceleration is zero when the velocity is parallel to the field. Moreover, it is straightforward to obtain

\[ \sum_{j=1}^{3} B_j m_j \ddot{x}_j = 0, \quad (3.2) \]

i.e., \( N \cdot \dot{r} = 0 \) with \( N_j = B_j m_j \). This means that an accelerated motion can only occur provided the acceleration is perpendicular to \( N \).

In order to solve Eq. 3.1, we look for solutions of the form \( \dot{r} = c \exp(i\omega t) \). This leads to the following eigenvalue problem:

\[ A \cdot c = \omega \cdot c, \quad (3.3) \]

where

\[ A = ie \begin{bmatrix} 0 & B_3/m_1 & -B_2/m_1 \\ -B_3/m_2 & 0 & B_1/m_2 \\ B_2/m_3 & -B_1/m_3 & 0 \end{bmatrix}. \quad (3.4) \]

The eigenvalues are \( \omega_{1,2} = \pm \omega_c \) and \( \omega_3 = 0 \), where [32]

\[ \omega_c = e \sqrt{\frac{B_1^2}{m_2 m_3} + \frac{B_2^2}{m_3 m_1} + \frac{B_3^2}{m_1 m_2}} \quad (3.5) \]

is the cyclotron frequency. Correspondingly, the cyclotron mass is given by [32]

\[ m_c = \frac{eB}{\omega_c} = \left( \frac{u_1^2}{m_2 m_3} + \frac{u_2^2}{m_3 m_1} + \frac{u_3^2}{m_1 m_2} \right)^{-1/2} \quad (3.6) \]

where the components of \( u = B/B \) are the direction cosines of the magnetic field.

The first two eigenvectors give rise to an elliptical motion in a plane perpendicular to \( N \). The period of such a closed orbit is \( T_c = 2\pi/\omega_c \), which is used as a unit of time in the following sections. The third eigenvalue corresponds to a uniform motion along the magnetic-field direction, i.e., parallel to the first eigenvector, \( c_1 = u \). In principle, the electron moves along a helix which is a superposition of the elliptical and linear motions. If the initial conditions lead to the excitation of the two motions, then the electron moves uniformly along \( N \), and the motion along \( B \) is a superposition of a uniform and an oscillatory motion. Figure 3.1 shows the main differences between the isotropic and anisotropic cases. In the first case, \( N \parallel B \) and the ellipse is a circle on a plane perpendicular to \( B \). In the second case, it is apparent that the ellipse is on a plane not perpendicular to the magnetic-field.
direction [33].

3.2.2 The anisotropic diamagnetic Kepler problem

When an electron with anisotropic mass, as described in the previous section, interacts with a single positive charge in the presence of a magnetic field $B = Bu$, the equations of motion read

$$m_j \ddot{x}_j = -\frac{e^2 x_j}{4\pi\epsilon r^3} - eB(\dot{r} \times u)_j,$$

(3.7)

with $\epsilon$ being the absolute value of the static dielectric permittivity of the medium through which the electron moves. This parameter is taken to be homogeneous and isotropic. By introducing new variables $\tilde{r} = r/\lambda$, $\tilde{t} = t/T_c$, and $\mu_j = m_j/m_c$, with

$$\lambda = \sqrt{\frac{\pi m_c}{\epsilon B^2}},$$

(3.8)

the equations of motion become

$$\mu_j \frac{d^2 \tilde{x}_j}{d\tilde{t}^2} = -\frac{\tilde{x}_j}{\tilde{r}^3} - 2\pi \left( \frac{d\tilde{r}}{d\tilde{t}} \times u \right)_j.$$  

(3.9)

3.2.3 The energy scale

The mechanical energy of the electron is given by

$$E = \sum_{j=1}^{3} \frac{m_j \dot{x}_j^2}{2} - \frac{e^2}{4\pi\epsilon r}.$$  

(3.10)
Hence, the dimensionless energy $\mathcal{E}_c = E/E_0$, with $E_0 = e^2/(4\pi\epsilon\lambda)$, is given by
\begin{equation}
\mathcal{E}_c = \sum_{j=1}^{3} \frac{\mu_j}{2} \left( \frac{d\tilde{r}_j}{dt} \right)^2 - \frac{1}{\tilde{r}}. \tag{3.11}
\end{equation}

Here we note that in order to compare with quantum mechanical approaches, the energy is better measured in units of the transversal Rydberg $R_y^* = e^4m_\perp/(32\pi^2e^2\hbar^2)$, and is given by $\mathcal{E}_q = E/R_y^*$. Therefore, by introducing the dimensionless measure of the magnetic-field strength $\gamma = \hbar eB/(2R_y^*m_\perp)$, we obtain
\begin{equation}
\mathcal{E}_c = \mathcal{E}_q\gamma^{-2/3} \left( \frac{\pi^2m_e}{2m_\perp} \right)^{1/3}. \tag{3.12}
\end{equation}

### 3.2.4 Equations for silicon

Silicon has a diamond crystal structure and the Cartesian co-ordinates are naturally chosen along the sides of a cubic crystallographic cell. The conduction band has six equivalent valleys along the $\Gamma$-$X$ lines, and the effective mass is diagonal in the Cartesian co-ordinate system. In each valley, the effective mass along the $\Gamma$-$X$ line is called the longitudinal mass and its value is denoted $m_{\parallel} = 0.9163m_0$, where $m_0$ is the bare electron mass. Moreover, the effective masses along the transversal directions are identical and their common value is given by $m_\perp = 0.1905m_0$. Therefore, the anisotropy is given by the ratio $\alpha = m_\perp/m_{\parallel} = 0.2079$. The relative dielectric permittivity is taken to be $\epsilon/\epsilon_0 = \epsilon_r = 11.4$.

In this work, the energy of the donor states refers to the conduction-band minimum and the intervalley coupling is disregarded. Thus, the role of each valley depends on the angle $\theta_B$ between the magnetic field and the longitudinal direction of the valley. Therefore, to simplify the calculations, one may choose the $z$-axis orientation along the longitudinal direction of the valley under question, with the $x$-$y$ plane containing the transversal directions. According to Sec. 3.2.1, $m_1 = m_2 = m_\perp$ and $m_3 = m_{\parallel}$, and the electron mass is given by
\begin{equation}
m_e = \frac{m_\perp}{\sqrt{\alpha \sin^2(\theta_B) + \cos^2(\theta_B)}}. \tag{3.13}
\end{equation}

If the magnetic field is applied along the (100) direction in silicon, then the magnetic field is parallel (perpendicular) to the longitudinal direction of two (four) valleys. Taking $\theta_B = 0^\circ$ and $\theta_B = 90^\circ$, the cyclotron mass is given by $m_e = m_\perp \approx 0.1905m_0$ and $m_e = \sqrt{m_\perp m_{\parallel}} \approx 0.4178m_0$, respectively. In contrast, when the field is along the (111) direction of silicon, the six valleys are equivalent and $\theta_B = \arccos(1/\sqrt{3}) \approx 54.7^\circ$. Then the cyclotron mass is $m_e = m_\perp\sqrt{3}/(2\alpha + 1) \approx 0.2773m_0$. 
3.2.5 Treatment of the Coulomb singularity

The numerical solution of Eq. 3.9 involves two main difficulties. On the one hand, the Coulomb force diverges as the inverse square of the distance to the origin. On the other hand, according to Eq. 3.11, the electron speed diverges as the square root of the distance to the origin. This implies that the magnetic force is very intense when the electron is nearby the impurity. These difficulties are of particular concern in this work, because the calculations focus on closed orbits described by the electron after launching from the vicinity of impurity centre. When the effective mass is isotropic, one may overcome the issues by introducing a rotating reference frame, semiparabolic co-ordinates, and a position-dependent time scaling as was utilised in Sec. 2.2. In the anisotropic case, as described below, the equations may be improved through a similar time-scaling transformation.

To regularize Eq. 3.11, one may introduce a scaled time $\tau$, such that

$$\frac{d\tilde{t}}{d\tau} = \tilde{r},$$

with $\tilde{t}(0) = 0$, i.e.,

$$\tilde{t} = \int_0^{\tau} \tilde{r}(\tau') d\tau'.$$

The transformed equation reads

$$\sum_{j=1}^{3} \mu_j \left( \frac{d\tilde{x}_j}{d\tau} \right)^2 = 1 + \mathcal{E} \tilde{r},$$

and shows that the new speed remains finite near the origin. In turn, Eq. 3.9 becomes

$$\mu_j \left( \frac{d^2\tilde{x}_j}{d\tau^2} - \frac{1}{2\tilde{r}} \frac{d\tilde{r}}{d\tau} \frac{d\tilde{x}_j}{d\tau} \right) = -\frac{\tilde{x}_j}{\tilde{r}^2} - 2\pi \sqrt{\tilde{r}} \left( \frac{d\tilde{r}}{d\tau} \times \mathbf{u} \right)_j.$$

Here the term associated with the Coulomb force presents a weaker singularity, and the term due to the magnetic field is negligible near the origin.

Regarding the initial conditions at $\tau = 0$, the singularity prevents us from considering launching the electron from the origin. Therefore, a small but finite value of the initial distance to the origin $\tilde{r}(0) = \tilde{r}_0$ should be used. The initial position is then given by $\tilde{r}(0) = \tilde{r}_0(\sin(\theta_r) \cos(\phi_r), \sin(\theta_r) \sin(\phi_r), \cos(\theta_r))$, where $\theta_r$ and $\phi_r$ are the polar and azimuthal angles. Accordingly, the initial velocity is taken as $\frac{d\tilde{r}}{d\tau}(0) = \tilde{u}_0(\sin(\theta_v) \cos(\phi_v), \sin(\theta_v) \sin(\phi_v), \cos(\theta_v))$, where, according to Eq. 3.16, the
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initial speed is given by

\[ \tilde{v}_0 = \sqrt{\frac{2(1 + \mathcal{E}_c \tilde{r}_0)}{\mu_\perp \sin^2(\theta_v) + \mu_\parallel \cos^2(\theta_v)}}. \]  

(3.18)

In the isotropic case, one may choose \( \phi_r = \phi_v \) and \( \theta_r = \theta_v \). This is because the dominant force near the origin is a central field. In silicon, the anisotropy presents axial symmetry and the first condition still holds. However, the polar angle undergoes fast changes near the origin. This means that an electron that is radially launched from the surface \( \tilde{r} = \tilde{r}_0 \) does not necessarily come from the origin (if negative values of \( \tau \) were considered). Therefore, for each value of \( \theta_v \), one must consider the special values of \( \theta_r \) that correspond to trajectories coming (essentially) from the impurity centre.

3.3 Numerical Results

To investigate the closed orbits of the electron, Eq. 3.17 is solved by launching the electron from a distance \( \tilde{r}_0 = 10^{-6} \). The isotropic case which corresponds to \( \alpha = 1 \) was dealt with in Chap. 2. Therefore, we concentrate here on the effects of anisotropy for different magnetic-field directions and electron energies. Included is a comparison to available experimental data.

3.3.1 Anisotropic case

To begin the analysis of the effects of anisotropy in silicon, we consider the case where the magnetic field is parallel to the longitudinal direction of the valley. In this case, because of the axial symmetry, the shape and duration of the orbits do not depend on the azimuthal launch angle \( \phi_v \), and one may limit the analysis to those values of the polar launch angle \( \theta_v \) between 0° and 90°.

The numerical results are obtained for \( \mathcal{E}_c = 0 \), by varying \( \theta_v \) in steps of 0.1°. Closed orbits who return to the impurity centre in less than five cyclotron periods (5\( T_c \)) only occur for polar launch angles very close to \( \theta_v = 90^\circ \). This means that the electron will not be able to return within 5\( T_c \) unless it departs along a direction with nearly minimum inertia.

The calculated orbits of donor electrons with energy \( \mathcal{E}_c = 0 \) in silicon subject to a magnetic field along the longitudinal direction of the valley are displayed in Fig. 3.2. In this case, the orbits may be analysed from a reference frame rotating at the Larmor frequency, and only those trajectories resembling the ones analysed for the
isotropic case in Fig. 2.2 are shown. One may note two main effects of anisotropy. On the one hand, except for the GT orbit, the anisotropy changes the duration of the closed orbits. On the other hand, since the spacing between the grid lines shown is 0.4 units, it is apparent that the anisotropy shrinks the orbits along the longitudinal direction of the valley.

The effects of the anisotropy in silicon should be stronger when the magnetic field is not parallel to the longitudinal direction of the valley. In such cases, the rotating reference frame is of little use, and one has to deal with three-dimensional orbits. To be concrete, we deal with the configuration where the magnetic field is applied along the (111) direction. Among the possibilities, this case is quite simple because the six valleys of the conduction band are equivalent (see Sec. 3.2.4). Numerical results were obtained for $E_c = 0$ and $\phi_v = 45^\circ$, by varying $\theta_v$ in $1^\circ$ steps over the range between $0^\circ$ and $180^\circ$. In this way, the electron is launched in the plane containing the z-axis and the magnetic-field direction. The three main closed orbits are shown in Fig. 3.3. The orbit displayed in Fig. 3.3(a) resembles the GT orbit shown in Fig. 3.2(a), and has a duration near the GT period. However, the plane perpendicular to $N$ is not horizontal, and the orbit is not exactly in the plane. In Figs. 3.3(b) and (c), one may note that trajectories are elongated in the direction of the magnetic field. When the electron is far from the impurity, the field affects the trajectory as to describe almost elliptical arcs whose plane is perpendicular to $N$. This is essentially the behaviour displayed by the helical trajectory in Fig. 3.1(b).
Figure 3.3: Closed orbits with $E_c = 0$, in silicon subject to a magnetic field along the (111) direction. Only the first three periods obtained for $\phi_v = 45^\circ$ are shown. The vertical line is the $z$-axis and the solid (dashed) arrow represents the magnetic field (the vector $N$ in Sec. 3.2.5, perpendicular to the shaded plane). The side of the shaded square is 0.8 units long.

3.3.2 Comparison with experiment

Up to now, we have seen that anisotropy affects the classical orbits of a conduction band electron in silicon subject to a magnetic field, and the effects depend on the angle between the magnetic-field direction and the longitudinal direction of the band valley. In this section, we look to make a comparison to the experimental data at hand. Thus, we consider a magnetic field strength of $B = 4$ T applied along the (111) direction, corresponding to the results reported in Fig. 3(a) of Ref. [19]. The cyclotron period is $T_c \approx 2.4766$ ps, and the oscillating part of the spectrum extends over a range of width $100 \text{cm}^{-1}$ above the ionisation threshold. As shown in Sec. 2.3, this corresponds to dimensionless values of the electron energy in the range $0 \leq E_c \leq 8.8$.

As discussed in Sec. 2.3.1, over this energy range, the periods and shapes of the orbits are expected to change noticeably. Consequently, the standard Fourier transform is not the best tool to obtain the periods of the main semiclassical orbits. Therefore, the reported periods should be considered as rough estimates: $T = 2.15, 5.05, 6.88, 8.30, \text{ and } 11.54$ ps. From the theoretical point of view, such periods might be found in some agreement with the periods calculated for $E_c = 4$ as was shown in Fig. 2.5(b) for the isotropic case.

In the anisotropic case of silicon with the magnetic field aligned with the (111) direction, the calculations for $E_c = 4$ are displayed in Fig. 3.4. The launching angles $\phi_v$ and $\theta_v$ vary between $0^\circ$ and $180^\circ$ with steps $5^\circ$ and $0.5''$, respectively. The dots are for orbits where the electron returns to the origin, re-entering a sphere of radius $0.01 \lambda$, centred at the origin. The wide lines correspond to the experimental periods $T/T_c \approx 0.87, 2.04, 2.78, 3.35, \text{ and } 4.66$. The theoretical results are found to be in
Figure 3.4: The periods of the closed orbits with $E_c = 4$, as a function of the azimuthal angle $\phi_v$, in silicon, with the magnetic field along the (111) direction. The dots correspond to the solutions of Eq. 3.9 with $\mu_1 = \mu_2 = 0.6870$ and $\mu_3 = 3.3043$. Only orbits where the electron re-enters a sphere of radius 0.01, centred at the origin, are included. The thick lines represent the experimental data peak positions in [19].

reasonable agreement with the experiment.

In fact, a series of closed-orbit periods that partially reproduce the peak positions in the Fourier transform of the experimental spectrum have been found. The agreement is expected to improve if the contribution of the different energy values is taken into account, at a much larger computational effort. Quantum-mechanical calculations should also contribute to a deeper understanding of the spectrum. Of course, new experimental measurements and data processing would be most valuable.

The shapes of some closed orbits corresponding to the points of Fig. 3.4 are shown in Fig. 3.5, for the case of an electron launched at an azimuthal angle of $\phi_v = 45^\circ$. After comparing with Fig. 3.3, it is apparent that the periods and shapes depend on
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![Figure 3.5](image1.png)  
**Figure 3.5:** As for Fig. 3.3, with $E_c = 4$ and $\phi_v = 45^\circ$.

![Figure 3.6](image2.png)  
**Figure 3.6:** As for Fig. 3.5, with $E_c = 4$ and $\phi_v = 135^\circ$.

the classical energy. By changing the value of $\phi_v$ to $135^\circ$, the orbits take the shapes as displayed in Fig. 3.6. It may be seen that the results depend of the launching azimuthal angle as well. We remark that the optical spectrum arises from the combination of the closed electron orbits associated with different energies and launching directions. Moreover, the contribution of each polar angle $\theta_v$ should be weighted by a factor $\sin(\theta_v)$, in order to compensate for the higher density of $\phi_v$ values. Nevertheless, Figs. 3.5 and 3.6 illustrate the electron dynamics related with a semiclassical interpretation of the experimental results.

3.4 Conclusion

In this chapter, we have successfully incorporated the effects of an anisotropic effective electron mass into the classical theoretical framework of the diamagnetic Kepler problem. The periods and the shapes of closed orbits have been shown to depend on the electron energy and magnetic-field direction. In the case of the magnetic field aligned along the longitudinal direction of the valley, due to axial symmetry, the orbits may be analysed from a reference frame rotating at the Larmor frequency as was utilised in Chap. 2. In this case, comparing to the isotropic case in Chap. 2, orbits are compressed along the longitudinal direction of the valley and the orbit periods are slightly different, except for the GT orbit which is unaffected due to being in the perpendicular plane. As the magnetic field is shifted away from the longitudinal direction of the valley, the rotating coordinate system is no longer useful, and the full three-dimensional representation of the orbits must be considered. Under this
configuration, orbits are elongated in the direction of the magnetic field and orbit periods are also effected by this elongation. The GT orbit, which remains in the perpendicular plane for the isotropic case and for the magnetic-field aligned with the longitudinal direction of the valley, is now pulled out of that perpendicular plane.

After this qualitative analysis of the periods and shapes of the orbits at the ionisation threshold ($E_c = 0$), we have chosen the classical energy near the middle of the energy range ($E_c = 4$) where the oscillations of the experimental absorption occur [19]. We have found reasonable agreement with available experimental data. However, as noted previously in Chap. 2, the Fourier transform of the optical spectra associated with donors in a semiconductor subject to a magnetic field of 4 T may not give the actual periods of relevant closed orbits. This is because the periods change substantially over the energy range of the investigated spectra [7].
Chapter 4

Diamagnetic Kepler problem in parallel electric and magnetic fields

4.1 Introduction

In Chaps. 2 and 3, we have only considered the case of an external magnetic field being applied to a hydrogenic electron system to observe quasi-Landau oscillations related to the classically chaotic motion of such electrons. In this chapter, we include an external static-electric-field applied in the same orientation as the applied magnetic field as shown in Fig. 4.1. In this specific orientation of the electric field, the rotational symmetry of the system about the magnetic-field axis remains intact, therefore, the theoretical framework of this problem results in the simple addition of an electric field term to the diamagnetic Kepler problem theory presented in Chap. 2. Consequently, the equations of motion include an additional parameter, the scaled field, which is a ratio of the electric to magnetic-field strengths. The integrals of motion of hydrogenic atoms in the presence of parallel magnetic and electric fields have been investigated by Beims et al. [34].

The main area of interest in the parallel fields system is that for a scaled field of zero, the system represents that of the classically-chaotic diamagnetic Kepler problem, however, at infinite scaled field, the system represents that of a pure electric field known as the Stark effect. In the Stark effect regime, the system is known to be classically regular due to the separability of the Hamiltonian [35–37], therefore, by systematically increasing the electric-field strength from the diamagnetic Kepler problem limit, the system can be observed moving from chaotic to regular dynamics. This was studied experimentally by König et al. [38] where the oscil-
Figure 4.1: The parallel field geometry for a hydrogenic electron system. The angles $\theta$ and $\phi$ show the polar and azimuthal launch angles respectively.

lations in the atomic spectrum of barium, and the associated Fourier transformed spectra, evolve as the electric-field strength was increased. They show a clear evolution in both the shape of the spectral oscillations, and the classical orbits identified in the Fourier transformed spectra, as the electric field is increased for a constant magnetic-field strength. For a strong electric-field, only one classical orbit exists in the system which is aligned parallel to the electric field. As the electric field is decreased from this Stark regime, Mao et al. [39] show how new orbits are created from the electric-field-induced orbit through what is referred to as a bifurcation process. At the specific scaled-field values at which a bifurcation occurs, a large increase in the peak amplitude associated with those orbits in the Fourier transformed experimental spectra is observed. Bifurcations have also been studied for the Stark system in lithium by Courtney et al. [36, 37] where the Coulomb potential differs to that of hydrogen due to the presence of extra electrons in the system. Therefore, the Hamiltonian for lithium in an electric field, unlike hydrogen, is inseparable, rendering the classical system as chaotic. They also observed, like Mao et al. [39], large increases in Fourier transform peaks around bifurcation points. Fielding et al. [40] show the application of a weak magnetic field significantly stabilizes the unstable electric-field-induced electron orbit associated with the Stark effect resulting in stronger peaks in the Fourier transformed spectra associated with this orbit and its
harmonics. As well as closed orbits, both periodic [41] and ionising orbits [42, 43] have also been investigated for the case of parallel magnetic and electric fields.

In this chapter, we start in Sec. 4.2 by deriving the classical equations of motion for a hydrogenic electron subject to parallel magnetic and electric fields. In Sec. 4.3 we utilise the equations of motion derived in Sec. 4.2 to investigate both the entire spectrum of closed orbits, and the four most stable orbits as identified by Du et al. [2], as the scaled field and scaled energy are varied, the latter specifically focussing on energies found to be pertinent to the case of silicon [19] as discussed in Chap. 2. A further investigation focusses on the mechanism by which orbits associated with quasi-Landau oscillations mix with the new electric-field-induced orbit as the scaled field is increased. The numerical results presented provide further understanding of how bifurcations lead to the strengthening of peaks in Fourier transformed spectra. Section 4.4 will then summarize the main results of the chapter.

4.2 Theory

The theory for parallel magnetic and electric fields is developed in much the same way as was done for the diamagnetic Kepler problem in Chap. 2, as for this specific field configuration, the system retains its rotational symmetry about the magnetic field axis. Therefore, assuming an isotropic electron mass, the equations of motion can be written in Cartesian co-ordinates \((x_j, j = 1, 2, 3)\) as

\[
m\ddot{x}_j = -\frac{e^2 x_j}{4\pi \epsilon r^3} - eB(\dot{r} \times u)_j - eF, \quad (4.1)
\]

where \(r\) is the radial vector, \(u = B/B\) is a vector whose components are the direction cosines of the magnetic field, and \(F\) is the electric field vector.

We orientate the magnetic and electric fields, without loss of generality, to be aligned along the z-axis. By once again scaling the distance and time by \(\tilde{r} = r/\lambda, \tilde{t} = t/T_c\), and utilising a rotating reference frame at \(\omega_c/2\) [10], the Lorentz force no longer depends on the velocity of the particle, and the equations of motion can now be written in the form

\[
\ddot{x}_j = -\frac{x_j}{r^3} - \pi^2(1 - \delta_{j,3}) \tilde{x}_j - f\tilde{x}_j, \quad (4.2)
\]

where \(\delta\) is the Kronecker delta, \(T_c = 2\pi/\omega_c\) is the cyclotron period, \(\omega_c = eB/m\) is the cyclotron frequency,

\[
\lambda = \sqrt[3]{\frac{\pi m}{eB^2}}. \quad (4.3)
\]
and
\[ f = \frac{4\pi^2 eF}{m\omega^2}\lambda, \]  
(4.4)
is the scaled field.

Equation 4.2 is related to the classical energy by
\[ E_c = \sum_{j=1}^{3} \frac{\dot{x}_j^2}{2} - \frac{1}{\tilde{r}} + \frac{\pi^2}{2} [\tilde{x}_1^2 + \tilde{x}_2^2] + f\tilde{x}_3, \]  
(4.5)
in scaled cylindrical co-ordinates \((\tilde{\rho}, \tilde{\phi}, \tilde{z})\), Eq. 4.5 can be written as
\[ E_c = \frac{\dot{\tilde{\rho}}^2}{2} + \left(\frac{L_3}{2\tilde{\rho}^2}\right)^2 + \frac{\dot{\tilde{z}}^2}{2} - \frac{1}{\tilde{r}} + \frac{\pi^2}{2} \tilde{\rho}^2 + f\tilde{z}, \]  
(4.6)
where \(L_3 = \tilde{\rho}^2 \tilde{\phi}\). We concentrate here only on the case of \(L_3 = 0\) and by introducing semiparabolic coordinates, \(u\) and \(v\), and scaled time \(\tau\), as utilised in Eqs. 2.13–2.18 of Chap. 2, Eq. 4.6 here may be simplified to
\[ \left(\frac{\dot{u}^2 + \dot{v}^2}{2}\right) - \frac{E_c (u^2 + v^2)}{4} + \frac{\pi^2 u^2 v^2 (u^2 + v^2)}{8} + \frac{f (u^4 - v^4)}{8} = \frac{1}{2}. \]  
(4.7)
The equations of motion in this semiparabolic coordinate system can be found from Eq. 4.7 using Hamilton’s equations, and are given by
\[ \ddot{u} = -\pi^2 \left[ \frac{u^3 v^2}{2} + \frac{u^2 v^4}{4} \right] + \frac{E_c u}{2} - \frac{f u^3}{2} \]  
(4.8)
and
\[ \ddot{v} = -\pi^2 \left[ \frac{u^2 v^3}{2} + \frac{u^4 v}{4} \right] + \frac{E_c v}{2} + \frac{f v^3}{2}. \]  
(4.9)
In the parallel magnetic and electric field case, as in the diamagnetic Kepler problem from Chap. 2, electrons are launched directly from the nucleus as the singularity at the origin no longer exists. The energy \(E_c\) is identically described in the same way as described for the diamagnetic Kepler problem in Eq. 2.22 of Chap. 2.

### 4.3 Numerical Results

In this section, we look to use the theoretical framework given in the previous section to explore the behaviour of the classical orbits as the scaled energy \(E_c\) and scaled field \(f\) are varied. In particular, we look to provide insight into possible effects that may be observable in the semiconductor environment. This differs from the atomic case most significantly due the oscillations in the experimental spectrum occurring
above the ionisation threshold [19], corresponding to positive values of the scaled energy. This is an energy region that has not been explored in detail in the literature due to it not being applicable to atomic investigations.

As was the case in the diamagnetic Kepler problem in Chap. 2, closed orbits are defined as those who return within 0.001λ of the nucleus within 5$T_c$. Due to the chaotic nature of the system, the polar launch angle is sampled at $\Delta \theta = 0.001^\circ$ intervals over a range of $\theta = 0–180^\circ$ with $\theta = 0^\circ$ corresponding to the alignment of the magnetic and electric fields. Due to the rotational symmetry of the system, the azimuthal launch angle can be ignored. Therefore, every closed orbit shown in this chapter belongs to an family of essentially an infinite number of closed orbits with varying azimuthal launch angle.

### 4.3.1 Varying scaled field

We begin our numerical investigation by studying the effects of increasing the scaled field at a fixed scaled energy of $E_c = 0$. Figure 4.2 shows the entire spectrum of closed orbits for the system at scaled field values of $f = 0, 0.01, 0.1$ and $1$. Figure 4.2 (a) is representative of a hydrogen atom in a static magnetic field which is a known chaotic system as was discussed in Chap. 2. The addition of a weak electric field aligned parallel to the applied magnetic field, as shown in Fig. 4.2 (b), only perturbs the system slightly. This is of particular interest in regards to the experimental technique of photothermal ionisation spectroscopy utilised in the measurements taken in silicon [19]. As we show here, the small electric field utilised in the experimental measurement is not large enough to significantly affect the underlying classical system. However, at this finite scaled field, orbits which were mirrored about $\theta = 90^\circ$ at $f = 0$ now have slightly different orbit periods due to launching either with or against the applied fields. Experimentally, this may be observed as peaks in the Fourier transformed spectra beginning to split due to these differences in orbit periods.

Increasing the strength of the electric field as depicted in Figs. 4.2 (c) and (d) leads to a more noticeable loss of symmetry around $\theta = 90^\circ$. As the electric field is increased, orbits migrate to launch angles closer to the direction of the applied electric field. This larger perturbation of the electron orbits has a stronger effect on the orbit periods as will be shown later. It is interesting to note that the application of the electric field produces a new closed orbit at $E_c = 0$ associated with the Stark effect. For instance, if $f = 1$ and $\theta = 0^\circ$, the period of a straight trajectory along the electric field is $T = 1.69443T_c$, with the maximum distance to the origin being
**Figure 4.2**: The return distance \( r_{\text{ret}} \) to the nucleus as a function of launch polar angle for scaled parallel fields (a) \( f = 0 \), (b) \( f = 0.01 \), (c) \( f = 0.1 \), and (d) \( f = 1 \). Data points are shaded according to their orbital period in the range \( 0-5T_c \) as indicated by the bar at the bottom of the figure.

\( r_{\text{max}} = \lambda \). As other orbits migrate further towards this part of the spectrum, they interact and mix together with this new orbit. The transition from the magnetic to the electric-field dominated atomic spectrum has been studied by König et al. [38] and will be investigated more thoroughly in a later section.

Table 4.1 presents values of the launching angle \( \theta \), orbit period, return distance, maximum distance, and bundle number \( N_{\text{bun}} \) for \( f = 0, 0.01, 0.1, \) and 1. In the absence of the electric field (\( f = 0 \)), the orbits correspond to the first four orbits from Fig. 8 of Ref. [2]. The orbit periods would correspond to peaks in the Fourier transform of experimental spectra showing a correspondence between classical orbits and oscillations observed in the spectrum. The maximum distance of the orbits are large enough to justify the use of classical physics to produce accurate results, and would also give an indication of the density of hydrogenic atoms required to consider every atom and associated orbits to be isolated. This was discussed in length in Chap. 2 when discussing different semiconductor candidates. The results given in Table 4.1 represent the local minima of the distance to the nucleus corresponding to
the bundle centres. As observed by the bundle numbers, orbits launched with their $z$-component parallel to the applied fields see an increase in stability the closer they migrate towards the applied fields. This increase in stability is shown in “Du2” with its bundle number increasing by a factor of 10 as it approaches a launch angle which is close to parallel with the external fields. Figures depicting the orbits detailed in Table 4.1 are shown in Figs. 4.3–4.16.

In Fig. 4.3, we see that as the scaled field is increased, the GT orbit (“Du1”) is pulled out of the perpendicular plane in the direction of the applied fields. As the scaled field increases, the orbit also becomes compressed in space as seen by the maximum distance in Table 4.1. This results in the reduction of the orbit as the scaled field is increased. Figures 4.5–4.8 show the behaviour of the orbit denoted as “Du2” from Chap. 2 as the scaled field is increased. At $f = 0$, the orbit launched in the hemisphere with its $z$-component aligned along the parallel fields, and the orbit launched in the opposite hemisphere, both share the same orbit period. However, as the scaled field is increased, the orbit launched in the hemisphere aligned with the parallel fields is stretched along the $z$-axis, thereby increasing its orbit period. Conversely, the orbit launched in the opposite hemisphere is compressed closer to the perpendicular plane, and its orbit period decreases with increasing scaled field. In the Fourier transform of experimental spectra, we expect this to manifest itself in the splitting of prominent peaks seen at low scaled-field values. The same behaviour is observed for the orbit denoted as “Du3” in Figs. 4.9–4.12. The only difference being that at high the high scaled field of $f = 1$, the orbit launched in the hemisphere aligned with the applied parallel fields no longer occurs. This is due to its launch angle having migrated so far as to be mixed with the electric-field-induced orbit created along the $z$-axis. A different behaviour is observed for orbit denoted as “Du4” in Figs. 4.13–4.16. At $f = 0$, this orbit is symmetric about the perpendicular plane, therefore, launching in either hemisphere results in the same orbit path. As the scaled field is increased, the symmetry about the perpendicular plane is broken as the orbit is rotated towards the direction of the parallel fields. However, the orbit still retains the same path regardless of the hemisphere from which it is launched. Therefore, the orbit periods remain the same and the peak in the Fourier-transformed experimental spectra would not show the same splitting with increased field as the orbits “Du2” and “Du3”.
<table>
<thead>
<tr>
<th>Orbit index</th>
<th>$f$</th>
<th>$\theta$ (degrees)</th>
<th>$T/T_c$</th>
<th>$r_{\text{ret}}/\lambda$</th>
<th>$r_{\text{max}}/\lambda$</th>
<th>$N_{\text{bun}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Du1</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.00</td>
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<td>90.00</td>
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<td>0.587368</td>
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<tr>
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<td>88.701</td>
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<tr>
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<td>$5.77 \times 10^{-9}$</td>
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<td>2872</td>
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<tr>
<td><strong>Du2</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
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<td>126.168</td>
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</tr>
<tr>
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<td></td>
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<td></td>
<td></td>
<td></td>
<td></td>
</tr>
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</tr>
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<td>2.04661</td>
<td>$6.97 \times 10^{-8}$</td>
<td>0.72474</td>
<td>408</td>
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</tbody>
</table>

Table 4.1: The polar launch $\theta$, period $T/T_c$, return and maximum distances, and the bundle number $N_{\text{bun}}$, for different values of the parallel scaled field $f$. Orbits are indexed according the convention outlined in Chap. 2.
Figure 4.3: The coordinate $z$ as a function of the cylindrical coordinate $\rho$ for the orbits evolving from the Garton-Tomkins orbit as the intensity of the parallel electric field is increased. The panels (a), (b), (c), and (d) are for dimensionless electric-field strength $f = 0, 0.01, 0.1,$ and 1, respectively. The point colour goes from red to blue as the electron describes the essentially closed path along the arrows shown. Colours representing the launch of the orbit in red are hidden when the curve overlaps itself.

Figure 4.4: The $x$ - $y$ view of the orbits in Fig. 4.3.

Figure 4.5: As for Fig. 4.3, but for the orbit denoted as “Du2”.

Figure 4.6: The $x$ - $y$ view of the orbits in Fig. 4.5. Arrows are omitted from (d) due to the size of the orbit, the path is the same as shown in (a), (b), and (c).
**Figure 4.7:** As for Fig. 4.3, but for the orbit denoted as “Du2”.

**Figure 4.8:** The $x$-$y$ view of the orbits in Fig. 4.7.

**Figure 4.9:** As for Fig. 4.3, but for the orbit denoted as “Du3”. The orbit at $f = 1$ has migrated its launch angle so far as to mix with the electric-field-induced orbit at $\theta = 0$.

**Figure 4.10:** The $x$-$y$ view of the orbits in Fig. 4.9.
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Figure 4.11: As for Fig. 4.3, but for the orbit denoted as “Du3”.

Figure 4.12: The $x$-$y$ view of the orbits in Fig. 4.11.

Figure 4.13: As for Fig. 4.3, but for the orbit denoted as “Du4”.

Figure 4.14: The $x$-$y$ view of the orbits in Fig. 4.13.
4.3.2 Varying scaled energy

In this section, rather than varying the scaled field at a fixed scaled energy as was covered in Sec. 4.3.1, we look to investigate the effect of holding the scaled field constant and varying the scaled energy over the range that was found to be applicable for the case of silicon in Chap. 2 [19]. Much of the work in the literature regarding elemental gases has been focussed in the region of $E_c \leq 0$. For the moment, we will focus on high field regime at $f = 1$, and vary the scaled energy over the range $E_c = 0–4$ in integer steps to observe how both the entire spectrum of orbits, and the individual orbits themselves vary over this range. A full set of results for both the entire spectrum of orbits, and first four orbits from Fig. 8 of Ref. [2] across all scaled field and scaled energy values considered in this chapter is given in Appendix A.

Figure 4.17 shows the spectrum of orbits as the scaled energy is increased in integer steps. Many of the orbits present at $E_c = 0$ no longer have periods less than $5T_c$ at higher energies, leaving only a few stable orbits. Orbit mixing no longer occurs as the energy is increased from $E_c = 0–1$ and, as it is increased to a value of $E_c = 4$, the electric-field-induced orbit disappears from the results as its period now exceeds the $5T_c$ threshold in the calculations.
Figure 4.17: The return distance \( r_{\text{ret}} \) to the nucleus as a function of launch polar angle for scaled field \( f = 1 \) and a scaled energy of (a) \( \mathcal{E}_c = 1 \), (b) \( \mathcal{E}_c = 2 \), (c) \( \mathcal{E}_c = 3 \), and (d) \( \mathcal{E}_c = 4 \).
### Table 4.2: The polar launch angle $\theta$, period $T$, return and maximum distances, and the bundle number $N_{\text{bun}}$, for different values of the classical energy $E_c$ at a fixed scaled field of $f = 1$. Orbits are indexed according to the convention outlined in Chap. 2.

<table>
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<tr>
<th>Orbit index</th>
<th>$E_c$</th>
<th>$\theta$ (degrees)</th>
<th>$T/T_c$</th>
<th>$r_{\text{ret}}/\lambda$</th>
<th>$r_{\text{max}}/\lambda$</th>
<th>$N_{\text{bun}}$</th>
</tr>
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<td>1.49 $\times 10^{-8}$</td>
<td>0.695772</td>
<td>1669</td>
<td></td>
</tr>
<tr>
<td>Du1</td>
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<td>6.10 $\times 10^{-9}$</td>
<td>0.804591</td>
<td>1108</td>
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<td>6.06 $\times 10^{-9}$</td>
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<td>87.589</td>
<td>2.69626</td>
<td>2.46 $\times 10^{-7}$</td>
<td>1.06528</td>
<td>29</td>
<td></td>
</tr>
</tbody>
</table>

...
Table 4.2 gives the values of the polar launch angle $\theta$, orbit period, return distance, maximum distance, and bundle number $N_{\text{bun}}$ for positive integer values of the classical scaled energy $E_c$ up to $E_c = 4$. Orbits displayed in Table 4.2 are shown in Figs. 4.18–4.31.

Figures 4.18 and 4.19 show the behaviour of the GT orbit (“Du1”) as the scaled energy is increased in integer steps. We see, as expected, that as the scaled energy is increased, the orbit expands in size and consequently takes longer to return to the nucleus. This is also seen by the maximum distance in Table 4.2 with the orbit at $E_c = 4$ showing a 72% increase in size over the orbit at $E_c = 0$. We also see from the figures that, as the scaled energy is increased, the launch angle shifts back towards the perpendicular plane. Therefore, increasing the scaled energy has the opposite effect on the classical electron orbits than increasing the scaled field.

Figures 4.20–4.23 show the behaviour of the orbit denoted as “Du2” as the scaled energy is incrementally increased. Both the orbits launched with their $z$-component with or against the applied parallel fields show significant changes in size, shape, and period over this scaled-energy range. However, as the increase in scaled energy leads to the launch angles of both variants of this orbit to migrate towards the perpendicular plane, their orbit periods begin to converge. For example, at $E_c = 0$, the difference in orbit period between the orbit launched with or against the applied fields was $0.12358T/T_c$, whereas at $E_c = 4$, this difference is reduced to $0.04788T/T_c$. In Sec. 4.3.1 we made the point that increasing the scaled field would lead to the splitting of peaks in the Fourier-transformed experimental spectra for this particular orbit. However, increasing the scaled energy acts to shift those split peaks back together as the orbits approach each other in the perpendicular plane.

Figures 4.24–4.27 show the behaviour of the orbit denoted as “Du3” as the scaled energy is increased. At $E_c = 0$, the orbit whose $z$-component of the launch direction was aligned with the applied parallel fields was not visible in the calculations as it had been mixed into the electric-field-induced orbit at $\theta = 0^\circ$. However, as we increase the scaled energy, this orbit emerges from the electric-field-induced orbit between $E_c = 1$–2 as its launch angle continues to move back towards the perpendicular plane. We would therefore expect in the Fourier-transformed experimental spectra for a peak associated with the electric-field-induced orbit to split as this orbit emerged between $E_c = 1$–2. The orbit with the $z$-component of the launch direction aligned against the applied fields shows the expected behaviour with the launch angle shifting towards the perpendicular plane, and the size and period of the orbit increasing with increasing scaled field.
Figures 4.28–4.31 show the behaviour of the orbit denoted as “Du4” as the scaled energy is increased in integer steps. This orbit differs from “Du2” and “Du3” due to the orbit rotating as the scaled field or energy are varied. Therefore, as the scaled energy is increased, the launch angle of the orbits launched in either hemisphere does not necessarily shift towards the perpendicular plane. This is indicated by focusing on the orbit launched against the applied fields at $E_c = 0$. As the scaled energy is increased, this orbits’ launch angle moves towards, and then past the perpendicular plane. Therefore, rather than the launch angles of this orbit moving towards the perpendicular plane, they actually move towards the GT orbit which has been pulled out of the plane. Apart from this difference, the orbits behave in the manner as observed for the other cases, with the orbit size and period increasing as the scaled energy is increased.

**Figure 4.18:** The coordinate $z$ as a function of the cylindrical coordinate $\rho$ for the orbits evolving from the Garton-Tomkins orbit as the intensity of the classical scaled energy is increased. The panels (a), (b), (c), (d), and (e) are for scaled energy values $E_c = 0, 1, 2, 3,$ and $4$, respectively. The point colour goes from red to blue as the electron describes the essentially closed path along the arrows shown. Colours representing the launch of the orbit in red are hidden when the curve overlaps itself.
Figure 4.19: The $x$-$y$ view of the orbits in Fig. 4.18.

Figure 4.20: As for Fig. 4.18, but for the orbit denoted as “Du2”.
Figure 4.21: The $x$-$y$ view of the orbits in Fig.4.20. Arrows are omitted from (a) due to the size of the orbit, the path is the same as shown in (b), (c), (d), and (e).

Figure 4.22: As for Fig.4.18, but for the orbit denoted as “Du2”.
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Figure 4.23: The $x$-$y$ view of the orbits in Fig. 4.22.

Figure 4.24: As for Fig. 4.18, but for the orbit denoted as “Du3”. Orbits at $E_c = 0$ and 1 are missing due to the orbit being mixed with the electric-field-induced orbit within this energy range.

Figure 4.25: The $x$-$y$ view of the orbits in Fig. 4.24.
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Figure 4.26: As for Fig. 4.18, but for the orbit denoted as “Du3”.

Figure 4.27: The x-y view of the orbits in Fig. 4.26.
Figure 4.28: As for Fig. 4.18, but for the orbit denoted as "Du4".

Figure 4.29: The $x$-$y$ view of the orbits in Fig. 4.28.
Figure 4.30: As for Fig. 4.18, but for the orbit denoted as “Du4”.

Figure 4.31: The $x$ - $y$ view of the orbits in Fig. 4.30.
4.3.3 Orbit mixing at intermediate and high fields

As was demonstrated earlier in Fig. 4.2 in Sec. 4.3.1, at scaled fields of approximately \( f = 1 \) an orbit orientated parallel to the applied magnetic and electric fields appears with a period less than \( 5T_c \). This orbit becomes more stable as the electric field is increased. As was also pointed out earlier, the orbits which are present at low fields migrate to launch angles close to parallel as the electric field is increased. Eventually, a field is reached in which these orbits begin to mix with the new electric-field-induced orbit and interesting features present themselves in the calculations. This section will focus on scaled fields of \( f = 0.8 \sim 1.18 \) at \( E_c = 0 \), increasing the field in 0.02 steps, in order to gain an understanding of how these orbits interact and mix with each other. At these scaled fields, in contrast to at weaker fields, there are large regions where closed orbits proliferate which explain the large increase in Fourier transform peak amplitudes around bifurcation points by Mao et al. [39] and Courtney et al. [36, 37].

Figure 4.32 depicts the system at angles \( \theta \sim 0^\circ \) for scaled fields of \( f = 0.8 \sim 0.98 \). At \( f = 0.8 \), orbits associated with quasi-Landau oscillations have migrated towards angles close to parallel from those shown earlier in Fig. 4.2(a) at \( f = 0 \). The orbit on the far left of all figures is the electric-field-induced orbit related to the Stark effect. The orbits which disappear between \( f = 0.8 \) and \( f = 0.82 \) in the launch angle region of \( \theta = 15 \sim 20^\circ \) are due to those orbits coming together, mixing, and then evolving to the point where no orbits return to within 0.001\( \lambda \) of the nucleus. This was observed by increasing the scaled field in smaller increments, with the results shown in Fig. 4.33. This discontinuity on the far right on the far right at \( f = 0.8 \) is due to the orbit period moving from below to above the \( 5T_c \) cutoff.
Figure 4.32: Return distance ($r_{\text{ret}}$) to the nucleus as a function of launch angle for scaled fields (a) $f = 0.8$, (b) $f = 0.82$, (c) $f = 0.84$, (d) $f = 0.86$, (e) $f = 0.88$, (f) $f = 0.9$, (g) $f = 0.92$, (h) $f = 0.94$, (i) $f = 0.96$, and (j) $f = 0.98$ at angles close to parallel to the applied fields.
Figure 4.33: Return distance ($r_{ret}$) to the nucleus as a function of launch angle for scaled fields (a) $f = 0.801$, (b) $f = 0.802$, (c) $f = 0.803$, (d) $f = 0.8035$, (e) $f = 0.804$, (f) $f = 0.805$, (g) $f = 0.806$, (h) $f = 0.807$, and (i) $f = 0.808$ at angles close to parallel to the applied fields.
CHAPTER 4. PARALLEL EXTERNAL FIELDS

Increasing the field to $f = 0.82$ leads to the orbits on the right of the figure shifting closer to parallel. The discontinuity no longer appears due to the higher field constricting the orbits further and therefore reducing their period below $5T_c$. Present in the figures are parabolas of different curvature with the same minimum point; these correspond to multiples ("harmonics") of the same orbit. The higher the harmonic, the more sensitive the orbit is to changes in initial launching angle, and therefore the sharper the parabola.

Increasing the field to $f = 0.84$, the orbits on the right-hand side of the figure are beginning to cluster together and become more stable as is illustrated when increasing the field again to $f = 0.86$. This effect is strongest in orbits with longer periods. A few orbits in the middle of the figure disappear between $f = 0.84$ and $f = 0.86$ due to same reasons as discussed previously for orbits disappearing between $f = 0.8$ and $f = 0.82$ and shown in Fig. 4.33.

At $f = 0.88$ we begin to see the overlapping of orbits and at $f = 0.9$ these orbits begin to mix, creating non-parabolic orbit dispersion patterns. There are quite a few discontinuities present in the calculations at these fields. However, as the field is increased further, these discontinuities evolve and represent the changing periods of the orbits around $5T_c$.

Increasing the field again to $f = 0.92$, previous discontinuities have been resolved due to the increase in field, and orbits previously seen as separated are now linked to one another. At $f = 0.94$, this creates a significant area of stability ranging over $\sim 15^\circ$. This represents quite a large range compared to the region covered by the most stable orbits at $f = 0$ (the GT orbit is stable over a launch angle range of $\sim 3^\circ$ as shown in Fig. 2.3 of Chap. 2). We would therefore expect such orbits to yield strong features in spectra, and their associated Fourier transform, at these fields due to the significant increase in the population of essentially closed orbits. The electric-field-induced orbit is also expanding its range of stability with increasing field, therefore we would expect to see it becoming more influential in experimental results.

At fields of $f = 0.96$ and $f = 0.98$, the electric-field-induced orbit continues to increase in stability and the orbits associated with quasi-Landau oscillations continue shifting to launch angles closer to parallel. This results in the mixing of these orbits and further extends the region of stability in the spectrum of orbits. More orbits are also entering the panels on the right side as they continue to migrate as the field increases. Discontinuities are still present and evolving with increasing
scaled field.

Figure 4.34 depicts the results at scaled fields of $f = 1 - 1.18$. At $f = 1$, the area of stability begins to contract backwards towards parallel as the orbits contributing to the right side of the large region of stability continue to shift towards parallel launch angles. Subsequently, we would expect the peaks observed in experimental data of Fourier transformed spectra to decrease in height as there is now a drop in the number of closed orbits over this scaled-field range.

At $f = 1.04$ the electric-field-induced orbit and its associated harmonics all diverge from stability in essentially the same manner. This is contrary to anything which has been observed in the calculations previously at other scaled fields as higher harmonics are expected to lose stability past as is observed in the GT orbit and other quasi-Landau-associated orbits. Experimentally we might expect the peaks in the Fourier transformed spectra to have equal intensity for peaks corresponding to each harmonic. Increasing the field again to $f = 1.06$, we have another orbit significantly increasing in stability as it approaches the electric-field-induced orbit.

At $f = 1.08$ this orbit mixes with the electric-field-induced orbit creating a larger region of stability for that particular harmonic than for the other two. Again, this may be able to be observed in Fourier transformed spectra in their respective peak intensities. At $f = 1.10$, this region of stability decreases as the orbit which has mixed continues shifting towards parallel launch angles.

At fields of $f = 1.12$ and $f = 1.14$, the approach of another quasi-Landau associated orbit to the electric-field-induced orbit is observed. As this new orbit approaches, it becomes increasingly more stable as seen by the widening of the parabola describing adjacent trajectories. The mixing of the orbit depicted at $f = 1.08$ in now unnoticeable at $f = 1.14$, as the region of stability of the electric-field-induced orbit contracts back towards its other harmonics.

At $f = 1.16$, the approaching orbit mixes with a different harmonic of the electric-field-induced orbit than was previously observed at $f = 1.08$. This mixing again leads to a large region of stability which may manifest itself in experimental measurements. Increasing the field again to $f = 1.18$, the mixing of the orbit with the electric-field-induced orbit follows the same pattern as was seen earlier in moving from $f = 1.08 - f = 1.10$. 
Figure 4.34: Return distance ($r_{ret}$) to the nucleus as a function of launch angle for scaled fields (a) $f = 1$, (b) $f = 1.02$, (c) $f = 1.04$, (d) $f = 1.06$, (e) $f = 1.08$, (f) $f = 1.10$, (g) $f = 1.12$, (h) $f = 1.14$, (i) $f = 1.16$, and (j) $f = 1.18$ at angles close to parallel to the applied fields.
Figure 4.35: Return distance \((r_{\text{ret}})\) to the nucleus as a function of launch angle for scaled field \(f = 20\).

Figure 4.35 shows all the closed orbits of the system for a scaled field \(f = 20\). At this strong field, all quasi-Landau-associated orbits have migrated to launch angles close to \(\theta = 0^\circ\) and are interacting with the electric-field-induced orbit and its associated harmonics. This represents a close to full transition from the chaotic regime at \(f = 0\) to the regular regime at \(f = \infty\). Therefore, we can conclude that the mixing of orbits which has been detailed represents the dynamics of the system shifting from the chaotic to regular regimes.

### 4.4 Conclusion

In this chapter, the closed orbits of an electron interacting with a positive unit charge in the presence of parallel magnetic and electric fields have been investigated. Such trajectories may manifest themselves in the optical spectrum of an atomic, or isotropic semiconductor system. In Sec. 4.2, the theory developed for the diamagnetic Kepler from in Chap. 2 is extended to include the effect of a constant electric field applied in the same direction as the applied magnetic field. For this special case, the system retains its rotational symmetry, and the method of obtain-
ing the classical equations of motion as utilised in Chap. 2 may be followed here with the addition of an electric-field term. The equations therefore have a strong resemblance to those for the diamagnetic Kepler problem, except now the equations depend on two parameters, the scaled energy $E_c$ and the scaled field $f$. The scaled field gives the ratio of the field strength between the magnetic and electric fields with $f = 0$ leading to the diamagnetic Kepler problem as discussed in Chap. 2, and $f = \infty$ representing the electron in a pure electric field (Stark effect). The calculations in this chapter show the evolution of the orbits reported by Du et al. [2] as the electric-field intensity is varied and the scaled energy is increased to small positive integer values. Small changes are seen for $f \leq 0.1$. However, at higher fields the orbits do undergo significant changes in size, shape, and duration.

In Sec. 4.3.1, we looked at the effect increasing the scaled field had on the overall spectrum of orbits and the four most important orbits as listed in Fig. 8 of Ref. [2]. It was found that as the scaled field was increased, the orbits broke their symmetry about the perpendicular plane ($\theta = 90^\circ$) at $f = 0$ and migrated in launch angle towards the electric-field direction. Subsequently, orbits which were launched with the $z$-component aligned with the applied parallel fields were stretched along the electric-field direction, and those whose $z$-component was aligned opposite to the applied fields became compressed along the electric-field direction. This led to a separation, in orbit period, between these two cases, and would therefore lead to the splitting of peaks in Fourier-transformed experimental spectra. However, this was only observed for orbits which, at $f = 0$, were not symmetric about the perpendicular plane. For the specific case of the orbit denoted as “Du4”, which is symmetric about the perpendicular plane at $f = 0$, this orbit was found to rotate towards the electric-field direction and no separation between launch angles with or against the applied parallel fields was observed. Therefore, for the peak which would be associated with this orbit in the Fourier transformed experimental spectra, no splitting would be observed. It was also shown that at high fields around $f = 1$, orbits associated with quasi-Landau oscillations had migrated in launch angle so far as to interact with the electric-field-induced orbit at angles close to $\theta = 0^\circ$.

Section 4.3.2 was dedicated to investigating how increasing the scaled energy, for a high scaled field of $f = 1$, in positive integer steps from $E_c = 0–4$, which was shown to be an important energy value in the case of silicon in Chap. 2, affected the complete spectrum of orbits and the four most important orbits investigated in Sec. 4.3.1. As the scaled energy was increased, the population of closed orbits identified in the complete spectrum of orbits decreased substantially. This is due to the increasing scaled-energy enlarging the size of the orbits, and therefore in-
creasing their period and decreasing their stability, resulting in many orbits being pushed above the $5T_e$ threshold or becoming unstable. It was also found that as the scaled energy was increased, the launch angles, in majority of cases, move towards the perpendicular plane and orbits are compressed to behave more as harmonics of the GT orbit. However, at some scaled-field values, orbits whose $z$-component of the launch direction was initially aligned against the applied fields move across the perpendicular plane. We therefore hypothesise that rather than launch angles moving towards the perpendicular plane, they are actually moving towards the GT-orbit orientation (which is pulled out of the perpendicular plane for finite values of the scaled field).

In Sec. 4.3.3, we revisited the phenomenon of quasi-Landau-associated orbits mixing with the electric-field-induced orbit at high scaled fields. In particular, we focussed on the scaled field region $f = 0.8 - 1.18$ to gain further insight into how these orbits interact and mix with each other. We observed in the calculations that this mixing of orbits produces comparatively large polar-launch-angle regions over which closed orbits proliferate which are not seen for lower scaled fields. We expect this large range of closed orbits to become more dominant in comparison to the rest of the orbit spectrum in experimental results as was observed for bifurcation points by [36, 37, 39]. Since this orbit mixing shows similar behaviour to the system at extreme electric-field strength, which is known to be a regular system, this orbit mixing may provide an indication of the system moving from chaotic to regular dynamics.
Chapter 5

Diamagnetic Kepler problem in crossed electric and magnetic fields

5.1 Introduction

In Chap. 4, we investigated the special case of including an electric-field parallel to the applied magnetic field. In that specific case, the rotational symmetry of the system was retained and calculations were relatively straightforward. In this chapter, we look at the case of applying an electric field in the plane perpendicular to the applied magnetic field as shown in Fig. 5.1. In this crossed-fields geometry, the rotational symmetry of the system is broken, and the calculation of closed classical orbits becomes much more cumbersome. The convention adopted by many authors has been to utilise the Kustaanheimo-Stiefel transformation [22, 23, 44–46] which expresses the close relationship between the three-dimensional hydrogen atom and a four-dimensional harmonic oscillator. This shifts the configuration space from three to four dimensions, and the phase space from six to eight dimensions, greatly increasing the complexity and computational expense over the methods previously utilised in Chaps. 2 and 4. However, in Sec. 5.2, we present a new simplified theoretical framework which builds on the conventions adopted for the diamagnetic Kepler problem and parallel-fields geometry to derive equations of motion for applied magnetic and electric fields of arbitrary orientation in semiparabolic coordinates. This allows us to calculate the closed classical orbits of the crossed-fields geometry in a much simpler manner than had been previously available.

Given the complicated nature of the calculations for the crossed-fields geometry, many of the investigations in the literature focus on the properties of specific sym-
Figure 5.1: The crossed field geometry for a hydrogenic electron system. The angles $\theta$ and $\phi$ show the polar and azimuthal launch angles respectively.

metries which exist in the system. Bartsch et al. [45] identify three inherent symmetries of the crossed-fields system. Firstly, reflection about the $x-y$ plane, secondly, the combination of time reversal and reflection about the $x-z$ plane, and lastly, the combination of the first and second symmetries. The symmetry about the $x-y$ plane is especially relevant given that for the diamagnetic Kepler problem, the most important classical orbit (the GT orbit) resides within this plane. Therefore, many investigations have been undertaken into the crossed-fields system within this plane, thereby simplifying calculations by reducing the dimensionality of the problem [44, 45, 47–51]. Neumann et al. [47] was the first to investigate, both experimentally and theoretically, the impact the addition of a perpendicular electric field has on the electron motion in the $x-y$ plane of the diamagnetic Kepler problem. They found that classically, as soon as the electric field is non-zero, the essentially infinite number of completely closed orbits who share the same properties, but varying azimuthal angle, reduces to only two completely closed orbits. However, the reduction in strength of the Fourier transform peak associated with those closed orbits is less dramatic, as orbits which are not necessarily closed, but pass close enough to the nucleus, still add to the oscillations in the spectrum. The oscillation strength is also adversely impacted by the crossed electric field due to the once essentially infinite family of closed orbits in the diamagnetic Kepler problem now having slightly
different periods. Therefore, quantum mechanically, there will be some deconstructive interference between orbits of the same family who have slightly different orbit periods. Milczewski et al. [44] utilised an approximation to the Hamiltonian for the crossed-fields system to provide insight into the chaotic properties and classical electron orbits of the system. Jaffe et al. [48, 49] focussed on the planar crossed-fields system, in particular, the classical ionisation of hydrogenic electrons and the study of periodic orbits. The study of ionisation and related classical orbits in the crossed-fields system has also been undertaken by various authors [52–54]. Wang et al. [50] consider the closed electron orbits in the $x–y$ plane and the various types of bifurcation processes that occur as the energy of the system is varied whilst remaining below the ionisation threshold. We perform a similar investigation using our new theoretical framework for energies at and above the ionisation threshold in Sec. 5.3.3 which provide some interesting new results.

The first experimental realization of a true crossed-fields hydrogenic system (small perturbations from the diamagnetic Kepler problem and Stark regime had been made previously) were made by Wiebusch et al. [55]. Their experimental spectra showed a strong correlation to second-order perturbation theory, however, the peaks observed in Fourier transformed spectra were not able to be ambiguously tied to specific classical closed orbits. Freund et al. [23] noted that, like had been discussed previously for the GT orbit in the $x–y$ plane, the peaks associated with closed classical orbits are much weaker in the crossed-fields geometry than for those systems with rotational symmetry as in Chaps. 2 and 4. To extract the periods of the weaker oscillations from experimental spectra, the authors developed the so-called “Chirped Fourier Transform” which allowed them to extract the Fourier transform peaks. They are then able to link the three simplest closed classical orbits to three of the most prominent peaks in the Fourier transformed spectra. Experiments have also been made in mediums other than hydrogen such as barium [16, 56] and rubidium [53]. Rao et al. [22] provide calculation methods for both the theoretical scaled spectra and the classical closed orbits of the system. They are then able to link every peak in the Fourier transformed theoretical spectra to a closed classical orbit and provide details of all 317 closed orbits identified [57]. Small deviations from the perpendicular fields configuration have also been investigated by Schleif et al. [58, 59] and the generalized case of arbitrary field orientations has been considered by Main et al. [60] with interesting results. However, their calculations use a quantum mechanical approach rather than the classical framework we present here.

In this chapter, we begin our investigation into the diamagnetic Kepler problem in crossed magnetic and electric fields by setting out the theoretical framework in
Sec. 5.2. Here, rather than adopting the convention of the Kustaanheimo-Stiefel transformation, we utilise scaled semiparabolic coordinates, and the choosing of appropriate initial conditions to soften the Coulomb singularity. The theory is also developed for the generalized case of applied magnetic and electric fields of arbitrary relative orientation. The equations of motion are then derived for the full 3D hydrogen atom. We then utilise these equations to analyse the special case of crossed magnetic and electric fields. In Sec. 5.3, three separate numerical investigations are undertaken. The first two, like the parallel-fields geometry in Chap. 4, focus on the scaled field (Sec. 5.3.1) and scaled energy (Sec. 5.3.2) dependence of both the entire spectrum of orbits, and the important closed orbits of the system respectively. In Sec. 5.3.3 we provide a detailed investigation into the first seven harmonics of the GT orbit which, unlike in the parallel-fields geometry, remain in the $x-y$ plane for any scaled field or scaled energy. This orbit is known to be the most significant in the analysis of experimental spectra in the crossed-fields geometry [44]. The important results from this chapter will then be summarized in Sec. 5.4.

5.2 Theory

In Chap. 4, we looked at the special case of an electric field applied in the same orientation as the applied magnetic field. In this section, we develop a new theoretical framework for hydrogen atom in static magnetic and electric fields of arbitrary orientation. We begin with the classical and non-relativistic motion equation which reads as

$$\frac{m}{2} \frac{d^2 \mathbf{r}}{dt^2} = -e \mathbf{F} - e \frac{d \mathbf{r}}{dt} \times \mathbf{B} - \frac{ke^2 \mathbf{r}}{r^3},$$

(5.1)

where $\mathbf{F}$ is the applied electric field and $k = 1/(4\pi \epsilon_0)$ is Coulomb’s constant. This is a conservative system and the electron energy is given by

$$\frac{m}{2} \left( \frac{d \mathbf{r}}{dt} \right)^2 + e \mathbf{F} \cdot \mathbf{r} - \frac{ke^2 \mathbf{r}}{r} = E.$$  

(5.2)

The motion equation in the case of the diamagnetic Kepler problem is numerically solved for the positive charge situated at the origin of coordinate system. In order to soften the singularity in the Coulomb term, semi-parabolic coordinates $u$ and $v$ and a scaled time $\tau$ are introduced [10, 11]. These coordinates are given by

$$x = \lambda uv \cos(\phi), \quad y = \lambda uv \sin(\phi), \quad \text{and } z = \frac{\lambda}{2} (u^2 - v^2),$$

(5.3)

where $\phi$ is the azimuth and

$$\lambda = \sqrt[3]{\frac{4\pi^2 ke^2}{m \omega_c^2}}.$$  

(5.4)
is a convenient unit of length. Therefore, the distance to the origin is \( r = \lambda (u^2 + v^2)/2 \). The scaled time is given by

\[
t = T_c \int_0^\tau \frac{r}{\lambda} \, d\tau ,
\]

where \( T_c = 2\pi/\omega_c \) is the cyclotron period.

To be concrete, the magnetic field is chosen along the positive direction of the \( z \) axis, i.e., \( B = (0, 0, B) \), with \( B > 0 \). The electric field will be given by \( F = F(\sin(\psi), 0, \cos(\psi)) \), where \( F \) is the intensity and \( 0 \leq \psi \leq \pi \). Utilising the scaling properties of the hydrogen atom, Eq. 5.1 may be written as

\[
\frac{d^2 \mathbf{r}}{dt^2} = \frac{\lambda}{T_c^2} \left[ -\frac{T_c e F}{\lambda m} \mathbf{a} - \frac{T_c e B}{m} \left( \frac{T_c}{\lambda} \frac{d\mathbf{r}}{dt} \right) \times \mathbf{b} - \frac{T_c^2 k e^2}{m \lambda^3} \frac{\lambda^2 r}{r^3} \right] ,
\]

where \( T_c^2 k e^2/(m \lambda^3) = 1 \), \( T_c e B/m = 2\pi \), \( \mathbf{a} = (\sin(\psi), 0, \cos(\psi)) \), \( \mathbf{b} = (0, 0, 1) \), and we define the scaled field as \( f = T_c^2 e F/(\lambda m) \). The motion equation now reads

\[
\frac{d^2 \mathbf{r}}{dt^2} = \frac{\lambda}{T_c^2} \left[ -f \mathbf{a} - 2\pi \left( \frac{T_c}{\lambda} \frac{d\mathbf{r}}{dt} \right) \times \mathbf{b} - \frac{\lambda^2 r}{r^3} \right] .
\]

As in Chap. 2, we utilise a notation where each dot over over a variable represents a derivative with respect to the scaled time \( \tau \). Therefore, from Eq. 5.5, we have

\[
i = \frac{T_c r}{\lambda} = \frac{T_c (u^2 + v^2)}{2} .
\]

Through the chain rule, we find

\[
\dot{r} = \lambda (u \dot{u} + v \dot{v})
\]

which leads to

\[
\ddot{r} = \frac{T_c \dot{r}}{\lambda} = T_c (u \ddot{u} + v \ddot{v}) .
\]

To obtain the equations of motion in semiparabolic coordinates, i.e. \( \ddot{u}, \ddot{v} \) and \( \ddot{\phi} \), we use the chain rule. To organize the equations efficiently, we use the Jacobian matrices. Therefore, on the one hand,

\[
\frac{dr}{dt} = \mathbb{J}^{-1} \frac{d}{dt} \begin{pmatrix} u \\ v \\ \phi \end{pmatrix} ,
\]

where \( \mathbb{J}^{-1} \) is the inverse of the Jacobian matrix.
where
\[
\mathbf{J}^{-1} = \begin{pmatrix}
\frac{\partial z}{\partial u} & \frac{\partial z}{\partial v} & \frac{\partial z}{\partial \phi} \\
\frac{\partial z}{\partial u} & \frac{\partial z}{\partial v} & \frac{\partial z}{\partial \phi} \\
\frac{\partial z}{\partial u} & \frac{\partial z}{\partial v} & \frac{\partial z}{\partial \phi}
\end{pmatrix} = \lambda \begin{pmatrix}
v \cos(\phi) & u \cos(\phi) & -uv \sin(\phi) \\
v \sin(\phi) & u \sin(\phi) & uv \cos(\phi) \\
u & -v & 0
\end{pmatrix}.
\] (5.12)

Hence,
\[
\frac{dr}{dt} = \frac{1}{t} \mathbf{J}^{-1} \begin{pmatrix}
\dot{u} \\
\dot{v} \\
\dot{\phi}
\end{pmatrix} = \frac{\lambda}{T_c r} \mathbf{J}^{-1} \begin{pmatrix}
\dot{u} \\
\dot{v} \\
\dot{\phi}
\end{pmatrix}.
\] (5.13)

On the other hand,
\[
\frac{d}{dt} \begin{pmatrix}
u \\
v \\
\phi
\end{pmatrix} = \mathbf{J} \frac{dr}{dt},
\] (5.14)

where
\[
\mathbf{J} = \begin{pmatrix}
v \cos(\phi) & v \sin(\phi) \frac{2r}{uv \lambda} & -\frac{2r}{uv \lambda} \\
v \cos(\phi) & v \sin(\phi) \frac{2r}{uv \lambda} & -\frac{2r}{uv \lambda} \\
-\sin(\phi) \frac{2r}{uv \lambda} & \cos(\phi) \frac{2r}{uv \lambda} & 0
\end{pmatrix}.
\] (5.15)

Therefore
\[
\begin{pmatrix}
\dot{u} \\
\dot{v} \\
\dot{\phi}
\end{pmatrix} = i \mathbf{J} \frac{dr}{dt}.
\] (5.16)

By utilising the chain rule again,
\[
\begin{pmatrix}
\ddot{u} \\
\ddot{v} \\
\ddot{\phi}
\end{pmatrix} = (i \mathbf{J} + i \mathbf{J}) \frac{dr}{dt} + \mathbf{J}^2 \frac{d^2 r}{dt^2}
\]
\[
= (r \mathbf{J} + r \mathbf{J}) \left( \frac{T_c}{\lambda} \frac{dr}{dt} \right) + \frac{r^2}{\lambda} \mathbf{J} \left\{ \frac{T_c}{\lambda} \frac{d^2 r}{dt^2} \right\}
\]
\[
= \frac{d(r \mathbf{J})}{d\tau} \left( \frac{T_c}{\lambda} \frac{dr}{dt} \right) + \frac{r^2}{\lambda} \mathbf{J} \left[ -f a - 2\pi \left( \frac{T_c}{\lambda} \frac{dr}{dt} \right) \times b - \frac{\lambda^2 r}{r^3} \right].
\] (5.17)

Now, using the result in Eq. 5.13, Eq. 5.17 becomes
\[
\begin{pmatrix}
\ddot{u} \\
\ddot{v} \\
\ddot{\phi}
\end{pmatrix} = \frac{1}{r} \frac{d(r \mathbf{J})}{d\tau} \mathbf{J}^{-1} \left( \begin{pmatrix}
\dot{u} \\
\dot{v} \\
\dot{\phi}
\end{pmatrix} - \frac{f r^2}{\lambda} \mathbf{J} a - \frac{2\pi}{\lambda} \mathbf{J} \left[ \mathbf{J}^{-1} \begin{pmatrix}
\dot{u} \\
\dot{v} \\
\dot{\phi}
\end{pmatrix} \right] \times b \right)
\]
\[
- \frac{\lambda r}{r},
\] (5.18)
CHAPTER 5. CROSSED EXTERNAL FIELDS

Eq. 5.13, the electron energy can be written as

\[
\begin{align*}
\frac{1}{r} \frac{d}{dx} r \mathbb{J}^{-1} \begin{pmatrix}
\dot{u} \\
\dot{v} \\
\dot{\phi}
\end{pmatrix} &= \frac{1}{u^2 + v^2} \begin{pmatrix}
(u^2 + \dot{v}^2 + v^2 \dot{\phi}^2)u \\
(u^2 + \dot{v}^2 + u^2 \dot{\phi}^2)v \\
-2 \left( \frac{\dot{u} v^2}{u} + \frac{\dot{v} u^2}{v} \right) \phi
\end{pmatrix},
\end{align*}
\]  
(5.19)

\[
\frac{f r^2}{\lambda} \mathbb{J} \mathbf{a} = \frac{f (u^2 + v^2)}{4} \begin{pmatrix}
v \cos(\phi) \sin(\psi) + u \cos(\psi) \\
u \cos(\phi) \sin(\psi) - v \cos(\psi) \\
- \frac{u^2 + v^2}{u v} \sin(\phi) \sin(\psi)
\end{pmatrix},
\]  
(5.20)

\[
\frac{2\pi r}{\lambda} \mathbb{J} \left( \mathbb{J}^{-1} \begin{pmatrix}
\dot{u} \\
\dot{v} \\
\dot{\phi}
\end{pmatrix} \times \mathbf{b} \right) = \pi \begin{pmatrix}
u u^2 \phi \\
u^2 v \phi \\
-(u^2 + v^2) \left( \frac{\dot{u}}{u} + \frac{\dot{v}}{v} \right)
\end{pmatrix},
\]  
(5.21)

and

\[
\frac{\lambda \mathbb{J} \mathbf{r}}{r} = \frac{1}{u^2 + v^2} \begin{pmatrix}
u \\
v \\
0
\end{pmatrix}.
\]  
(5.22)

From Eqs. 5.18–5.22, each second derivative is easily collected and given by

\[
\ddot{u} = \frac{(u^2 + \dot{v}^2 + v^2 \dot{\phi}^2 - 1)u}{u^2 + v^2} - \frac{f (u^2 + v^2)}{4} [v \cos(\phi) \sin(\psi) + u \cos(\psi)]
\]  
(5.23)

\[
\ddot{v} = \frac{(u^2 + \dot{v}^2 + u^2 \dot{\phi}^2 - 1)v}{u^2 + v^2} - \frac{f (u^2 + v^2)}{4} [u \cos(\phi) \sin(\psi) - v \cos(\psi)]
\]  
(5.24)

and

\[
\ddot{\phi} = - \frac{2 \dot{\phi}}{u^2 + v^2} \left( \frac{\dot{u} u^2}{u} + \frac{\dot{v} v^2}{v} \right) + \frac{f (u^2 + v^2)^2}{4 u v} \sin(\phi) \sin(\psi)
\]  
+ \pi (u^2 + v^2) \left( \frac{\dot{u}}{u} + \frac{\dot{v}}{v} \right),
\]  
(5.25)

Returning to the electron energy equation in Eq. 5.2, and utilising the result in Eq. 5.13, the electron energy can be written as

\[
\frac{m \lambda^2}{2 T^2 c^2} \left( \ddot{u} \quad \ddot{v} \quad \ddot{\phi} \right) \mathbb{J}^{-1} \mathbb{J}^{-1} \begin{pmatrix}
\dot{u} \\
\dot{v} \\
\dot{\phi}
\end{pmatrix} + e \mathbf{F} \cdot \mathbf{r} - \frac{k e^2}{r} = E,
\]  
(5.26)

where \( \mathbb{J}^{-1} \) is the transpose of \( \mathbb{J}^{-1} \). Eq. 5.26 can therefore be expressed as

\[
\frac{2}{(u^2 + v^2)^2} \left[ (u^2 + v^2)(\ddot{u}^2 + \ddot{v}^2) + u^2 v^2 \ddot{\phi}^2 \right] + \frac{T^2_c e^2}{m \lambda^2} \mathbf{a} \cdot \mathbf{r} - \frac{T^2_c k e^2}{m \lambda^2 r} = E_c,
\]  
(5.27)
or completely in semiparabolic coordinates as
\[
\frac{2}{(u^2 + v^2)^2} \left[ (u^2 + v^2)(\dot{u}^2 + \dot{v}^2) + u^2v^2\dot{\phi}^2 \right] \\
+ \frac{f}{2} [2uv \cos(\phi) \sin(\psi) + (u^2 - v^2) \cos(\psi)] - \frac{2}{u^2 + v^2} = E_c, \tag{5.28}
\]
where \( E_c = T_c^2 E / (m\lambda^2) \). Eq. 5.28 can be re-arranged to give
\[
\frac{\dot{u}^2 + \dot{v}^2 - 1}{u^2 + v^2} = - \frac{u^2v^2\dot{\phi}^2}{(u^2 + v^2)^2} - \frac{f}{4} [2uv \cos(\phi) \sin(\psi) + (u^2 - v^2) \cos(\psi)] + \frac{E_c}{2}. \tag{5.29}
\]
After introducing
\[
\omega = \frac{1}{\omega_c} \frac{d\phi}{dt} = \frac{\dot{\phi}}{\omega_c t} = \frac{\lambda t}{2\pi r} = \frac{\dot{\phi}}{\pi (u^2 + v^2)}, \tag{5.30}
\]
and substituting the result of Eq. 5.29 into the equations of motion in Eqs. 5.23–5.25, we obtain the final equations of motion to be
\[
\ddot{u} = u \left[ -\pi^2 \omega^2 u^2 v^2 - \frac{f}{4} [2uv \cos(\phi) \sin(\psi) + (u^2 - v^2) \cos(\psi)] \\
+ \frac{E_c}{2} + \pi^2 \omega^2 v^2 (u^2 + v^2) \right] - \frac{f(u^2 + v^2)}{4} [v \cos(\phi) \sin(\psi) + u \cos(\psi)] \\
- \pi^2 \omega uv^2 (u^2 + v^2) \\
= u \left[ -\pi^2 \omega u^2 v^2 - \pi^2 \omega (1 - \omega) v^4 + \frac{E_c}{2} \right] - \frac{f}{4} [(3u^2 + v^2) v \cos(\phi) \sin(\psi) \\
+ 2u^3 \cos(\psi)], \tag{5.31}
\]
\[
\ddot{v} = v \left[ -\pi^2 \omega^2 u^2 v^2 - \frac{f}{4} [2uv \cos(\phi) \sin(\psi) + (u^2 - v^2) \cos(\psi)] \\
+ \frac{E_c}{2} + \pi^2 \omega^2 u^2 (u^2 + v^2) \right] - \frac{f(u^2 + v^2)}{4} [u \cos(\phi) \sin(\psi) - v \cos(\psi)] \\
- \pi^2 \omega u^2 v(u^2 + v^2) \\
= v \left[ -\pi^2 \omega u^2 v^2 - \pi^2 \omega (1 - \omega) u^4 + \frac{E_c}{2} \right] - \frac{f}{4} [(3v^2 + u^2) u \cos(\phi) \sin(\psi) \\
- 2v^3 \cos(\psi)], \tag{5.32}
\]
and
\[ \dot{\omega} = \frac{\ddot{\phi}}{\pi(u^2 + v^2)} - \frac{2\omega(u\dot{u} + v\dot{v})}{u^2 + v^2} \]
\[ = \frac{1}{\pi(u^2 + v^2)} \left[ -2\pi\omega \left( \frac{\dot{u}v^2}{u} + \frac{\dot{v}u^2}{v} \right) + \frac{f(u^2 + v^2)^2}{4uv} \sin(\phi) \sin(\psi) \right] \]
\[ + \pi(u^2 + v^2) \left( \frac{\ddot{u}}{u} + \frac{\ddot{v}}{v} \right) - \frac{2\omega(u\dot{u} + v\dot{v})}{u^2 + v^2} \]
\[ = \frac{f(u^2 + v^2)}{4\pi uv} \sin(\phi) \sin(\psi) + (1 - 2\omega) \left( \frac{\dot{u}}{u} + \frac{\dot{v}}{v} \right). \quad (5.33) \]

Finally, the energy equation (Eq. 5.29) may be rewritten as
\[ \frac{\dot{u}^2 + \dot{v}^2 - 1}{u^2 + v^2} = -\pi^2 \omega^2 u^2 v^2 - \frac{f}{4} [2uv \cos(\psi) \sin(\phi) + (u^2 - v^2) \cos(\psi)] + \frac{\mathcal{E}_c}{2} \]  
(5.34)

or
\[ \frac{\dot{u}^2 + \dot{v}^2}{2} + \frac{\pi^2}{2} \omega^2 u^2 v^2 (u^2 + v^2) + \frac{f}{8} [2uv(u^2 + v^2) \cos(\phi) \sin(\psi) \]
\[ + (u^4 - v^4) \cos(\psi)] - \frac{\mathcal{E}_c(u^2 + v^2)}{4} = \frac{1}{2}. \quad (5.35) \]

The electron launches essentially from the origin. Theoretically, since the present approach does not include relativistic effects, the initial distance to the origin cannot be too small. For moderate energy values, i.e., for \(|E| \ll mc^2\), such a distance should be much larger than \(2ke^2/(mc^2) \approx 5.6\) fm. This is fairly small in comparison with the size of the hydrogen atom. Therefore, in the numerical calculations, one may take the initial position as \(u = v = 0\).

The direction of the initial velocity is given by the polar angle \(\theta\) and the azimuth \(\phi\). Since the initial electron position is the origin of coordinates, Eq. 5.35 leads to \(\ddot{u} + \ddot{v} = 1\). Therefore, one may take \(\dot{u} = \cos(\theta/2)\) and \(\dot{v} = \sin(\theta/2)\). The singularity in Eq. 5.33 is avoided by taking \(w = 1/2\) at \(t = 0\). Thus the initial value of \(\dot{w}\) is \(f \sin(\psi) \sin(\phi)/(2\pi \sin(\theta))\).

This method of scaling the equations and utilizing semi-parabolic coordinates has been used in the special cases of pure magnetic fields detailed in Chap. 2 and parallel electric and magnetic fields detailed in Chap 4 for several decades. In the case of crossed electric and magnetic fields, due to the loss of rotational symmetry in the system, this method has been confined to analysing the 2D hydrogen atom [49, 51, 61]. In the 3D hydrogen atom, other methods such as combining the Kustaanheimo-Stiefel transformation with a time-dilation variable in a four-dimensional represen-
tation have been required. Here we show that scaling of the equations, and utilizing semiparabolic coordinates, which had been predominantly limited to use in special cases with rotational symmetry, can also be generalized for arbitrary orientation of electric and magnetic fields in the 3D hydrogen atom.

5.3 Numerical results

The crossed-fields geometry lacks the rotational symmetry of the pure magnetic field and parallel fields cases and therefore calculations should be performed for different values of the polar launch angle $\theta$ and the azimuthal launch angle $\phi$. While $\theta$ varies from $0^\circ$ to $180^\circ$, $\phi$ goes from $0^\circ$ to $360^\circ$. We first show that our simplified theoretical framework, detailed in Sec. 5.2, is able to produce the same results as those reported by Rao et al. [22]. To calculate the orbits displayed in Fig. 4 of that work, we must convert the energy and electric-field values to the units utilized in Sec. 5.2. The values of $E_c$ and $f$ in Ref. [22] should be multiplied by $(2\pi)^{2/3}$ and $(2\pi)^{4/3}$, respectively.

The calculations for $E_c = -1.9971777136500313$ and $f = 0.7946397341001873$ yield the orbits displayed in Fig. 5.2. The shapes of the orbits are in good agreement with Figs. 4(a) and 4(b) of Ref. [22]. The sizes of the orbits in the present calculation are smaller due to the use of a unit length which is $(2\pi)^{2/3}$ times larger.

The overall dependence of the launching direction and duration of the closed orbits on the strength of the electric field is displayed in Fig. 5.3. As the field strength
increases from panel (a) to (c), the dependence of the polar angles and duration of closed orbits on the azimuthal angle becomes more apparent. The reflection symmetry with respect to the $x$-$y$ plane, i.e., $\theta = 90^\circ$, is quite evident. Moreover, the orbits of shorter duration are launched on the symmetry plane and evolve from the GT orbits. The evolution may be understood by analysing Fig. 5.4, where the two orbits having minimum return distance and displayed for $f = 0.01$, $f = 0.1$, and $f = 1$. The duration of the closed orbits in panels (a), (c), and (e) is less than $\frac{2}{3}T_c$. As the electric-field strength increases, both the duration and the size of the orbit decrease. The orbits in panels (b), (d), and (f) last more than $\frac{2}{3}T_c$ and display the opposite dependence on the field strength. This azimuthal dependence of the GT orbit will be discussed in much more detail in Sec. 5.3.3.

It should be stressed that the theoretical framework developed in Sec. 5.2 is not appropriate for the study of orbits launched near either $\theta = 0^\circ$ or $\theta = 180^\circ$ in crossed fields. Therefore, orbits of this kind that have been reported by Rao et al. [22, 57] have not been obtained here. Nevertheless, such orbits are not very stable and should not manifest themselves in the optical spectra.
Figure 5.3: The relation between the polar launch angle $\theta$ and the azimuthal launch angle $\phi$ of essentially closed orbits of an electron with $E_c = 0$, in the presence of crossed magnetic and electric fields along the directions of the $z$ and $x$ axes, respectively. Panels (a) – (c) are for electric-field strength $f = 0.01$, $f = 0.1$, and $f = 1$, respectively. Orbits whose scaled returning distance, $r_{ret}/\lambda$, is larger than (a) 0.00001, (b) 0.0001, and (c) 0.001 are not shown.
Figure 5.4: The shapes of the planar closed orbits that evolve from the Garton-Tomkins orbit in the crossed fields, for $E_c = 0$, where panels (a) and (b) are for $f = 0.01$, (c) and (d) $f = 0.1$, and (e) and (f) $f = 1$. 

Panel (a): $T \approx 0.6660 T_c$, $\theta = 90^\circ$, $\phi \approx 300.10^\circ$.

Panel (b): $T \approx 0.6674 T_c$, $\theta = 90^\circ$, $\phi \approx 119.90^\circ$.

Panel (c): $T \approx 0.6596 T_c$, $\theta = 90^\circ$, $\phi \approx 300.90^\circ$.

Panel (d): $T \approx 0.6737 T_c$, $\theta = 90^\circ$, $\phi \approx 119.10^\circ$.

Panel (e): $T \approx 0.5980 T_c$, $\theta = 90^\circ$, $\phi \approx 308.20^\circ$.

Panel (f): $T \approx 0.7373 T_c$, $\theta = 90^\circ$, $\phi \approx 110.30^\circ$. 

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5.3.1 Varying scaled field for specific azimuthal launch angles

We first consider the case where the electron is launched on the vertical semiplane given by \( y = 0 \) and \( x \geq 0 \), i.e., \( \phi = 0^\circ \). The parameters of the orbits that evolve from the first four orbits from Fig. 8 of Ref. [2] ("Du1"–"Du4") in the absence of the electric field are given in Table 5.1.

<table>
<thead>
<tr>
<th>Orbit index</th>
<th>( f ) (degrees)</th>
<th>( T/T_c )</th>
<th>( r_{ret}/\lambda )</th>
<th>( r_{max}/\lambda )</th>
<th>( N_{bun} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Du1</td>
<td>0.00</td>
<td>90</td>
<td>0.666667</td>
<td>1.23x10^-8</td>
<td>0.587368</td>
</tr>
<tr>
<td></td>
<td>0.01</td>
<td>90</td>
<td>0.666003</td>
<td>2.30x10^-6</td>
<td>0.586742</td>
</tr>
<tr>
<td></td>
<td>0.10</td>
<td>90</td>
<td>0.660125</td>
<td>2.2x10^-4</td>
<td>0.581168</td>
</tr>
<tr>
<td></td>
<td>1.00</td>
<td>90</td>
<td>0.607804</td>
<td>1.4x10^-2</td>
<td>0.530252</td>
</tr>
<tr>
<td>Du2</td>
<td>0.00</td>
<td>53.832</td>
<td>1.57087</td>
<td>1.11x10^-7</td>
<td>0.707068</td>
</tr>
<tr>
<td></td>
<td>0.01</td>
<td>53.793</td>
<td>1.56928</td>
<td>8.35x10^-6</td>
<td>0.706661</td>
</tr>
<tr>
<td></td>
<td>0.10</td>
<td>53.472</td>
<td>1.55474</td>
<td>7.52x10^-4</td>
<td>0.702828</td>
</tr>
<tr>
<td></td>
<td>1.00</td>
<td>52.085</td>
<td>1.37526</td>
<td>1.8x10^-2</td>
<td>0.652981</td>
</tr>
<tr>
<td>Du3</td>
<td>0.00</td>
<td>42.810</td>
<td>2.58192</td>
<td>7.12x10^-8</td>
<td>1.10748</td>
</tr>
<tr>
<td></td>
<td>0.01</td>
<td>42.770</td>
<td>2.57934</td>
<td>2.22x10^-5</td>
<td>1.10667</td>
</tr>
<tr>
<td></td>
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</tr>
<tr>
<td></td>
<td>1.00</td>
<td>40.993</td>
<td>2.25026</td>
<td>1.8x10^-4</td>
<td>0.989591</td>
</tr>
<tr>
<td>Du4</td>
<td>0.00</td>
<td>63.650</td>
<td>2.14513</td>
<td>8.03x10^-8</td>
<td>0.642937</td>
</tr>
<tr>
<td></td>
<td>0.01</td>
<td>63.647</td>
<td>2.14089</td>
<td>6.17x10^-7</td>
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<tr>
<td></td>
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<td>1.84521</td>
<td>4.3x10^-3</td>
<td>0.625781</td>
</tr>
</tbody>
</table>

Table 5.1: The launching angle \( \theta \), period \( T \), return and maximum distances, and the bundle number \( N_{bun} \), for different values of the crossed electric-field intensity \( f \). The launching azimuth is \( \phi = 0^\circ \). Values of \( N_{bun} \) become zero when no orbits of that type return within 0.001\( \lambda \) of the nucleus.

Unlike the case of parallel fields, the polar launch angle remains relatively unchanged as the scaled field is increased. At high scaled fields, the classical orbits which are the most stable at low scaled fields, in most cases, no longer return enough to the nucleus to be considered as closed orbits (as denoted by \( N_{bun} = 0 \)). Curiously, the orbit denoted “Du3” shows a higher stability at \( f = 1 \) than for lower scaled fields. Note that these results are only for the plane \( \phi = 0^\circ \) and orbits with \( N_{bun} = 0 \) may return to the nucleus in other azimuthal planes. This will be explored further in Sec. 5.3.3 for the case of the GT orbit ("Du1") and its harmonics.

Figure 5.5 depicts how the spectrum of orbits evolve as the scaled field is varied for \( \phi = 0^\circ \). As was the case for parallel fields, a weak electric fields only yields a small perturbation in the results as was seen in Table 5.1. As the field is increased...
further, fewer orbits return close to the nucleus. This is seen by the relative absence of orbits returning with a distance of 0.0002λ in this case compared to the parallel fields case in Chap. 4. In the crossed-fields configuration, the plane containing the orbit which is identified as the GT orbit at $f = 0$ is now parallel to the electric field which changes the behaviour of this orbit substantially. At $f = 0.1$ it is seen that the first harmonic is no longer returning as close to the nucleus as at lower fields, and at $f = 1$ it no longer return to within the 0.001λ threshold. Figures depicting the orbits detailed in Table 5.1 are presented in Figs. 5.6–5.13. Due to the symmetry of the crossed fields system about the $x$-$y$ plane, only the orbits who are launched with their $z$-component aligned along the magnetic field direction will be shown.
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**Figure 5.6:** The coordinate $z$ as a function of the cylindrical coordinate $\rho$ for the orbits evolving from the Garton-Tomkins orbits ("Du1") as the intensity of the crossed electric field is increased. The electron launches in a vertical plane containing the electric field direction, i.e., $\phi = 0^\circ$. The panels (a), (b), (c), and (d) are for dimensionless electric-field strength $f = 0, 0.01, 0.1$, and $1$, respectively.

**Figure 5.7:** The $x$-$y$ view of the orbits in Fig. 5.6.

**Figure 5.8:** As for Fig. 5.6, but for the orbit denoted as "Du2". Here, unlike in previous chapters, $\rho$ is now represented as an absolute value due to the different theoretical framework.

**Figure 5.9:** The $x$-$y$ view of the orbits in Fig. 5.8.
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Figure 5.10: As for Fig. 5.8, but for the orbit denoted as "Du3".

Figure 5.11: The x-y view of the orbits in Fig. 5.10.

Figure 5.12: As for Fig. 5.8, but for the orbit denoted as "Du4".

Figure 5.13: The x-y view of the orbits in Fig. 5.12.
In Fig. 5.6 we see that, as the scaled field is increased, the GT orbit ("Du1") remains in the $x$-$y$ plane ($\theta = 90^\circ$) due to the electric field now being applied in this same plane. However, this leads to this particular harmonic of the GT orbit to not form a closed orbit as is evident in Fig. 5.7 (d). As was the case for the parallel fields case in Chap. 4, the increasing scaled field leads to the orbit becoming more confined in space, therefore reducing the period of the orbit.

Figures 5.8 and 5.9 show the evolution of the orbit denoted as "Du2" as the crossed electric field is increased in intensity. Due to the theoretical framework for the crossed fields case utilising slightly different definitions than in previous chapters, the coordinate $\rho$ must be positive. Therefore, the orbit follows the first half of its trajectory in the same manner as was seen previously, however, at the $\rho = 0$ plane it is reflected. Unlike the GT orbit discussed in the previous paragraph, this orbit’s launch angle does change, albeit slightly when compared to the large changes observed in the parallel-fields case. At high fields, this orbit also develops different launch and return polar angles, as demonstrated in Fig. 5.8 (d). As was the case for the GT orbit, the size and therefore the period of the orbits decreases with increasing scaled-field intensity.

The behaviour of the orbit denoted as “Du3” is shown in Figs. 5.10 and 5.11 where many of the same characteristics as discussed for “Du2” are observed. However, this orbit returns closer to the nucleus at $f = 1$ than for $f = 0.1$ as shown in Table 5.1. This is the only instance of this occurring for any of the four orbits studied in detail in this section. The orbit denoted as “Du4” is shown in Figs. 5.12 and 5.13. As was the case for “Du3”, this orbit behaves in much the same manner as was discussed for “Du2”. However, unlike the other orbits whose launch angles moved slightly towards the electric field orientation as the intensity was increased, the fourth orbit shows a slight shift in towards the direction of the applied magnetic field at high scaled fields.

Earlier we noted that at high scaled field ($f = 1$) that the orbits which dominate at low scaled field are not considered as closed orbits at high field. However, Fig. 5.5 (d) shows quite a few quite stable orbits particularly around $\theta = 90^\circ$. These orbits have been identified as the 4th (green) and 7th (blue) harmonics of the GT orbit ("Du1"). These orbits show a stability comparable to that of the principle GT orbit at low scaled field with the 4th harmonic having a bundle number of $N_{\text{bun}} = 2836$ and the 7th harmonic $N_{\text{bun}} = 2518$. These will be explored in more detail in Sec. 5.3.3.

Next we consider the case in which the electron is launched in the plane perpendicular to the applied electric field, i.e., $\phi = 90^\circ$. Table 5.2 and Fig. 5.14 show how
<table>
<thead>
<tr>
<th>Orbit index</th>
<th>$f$</th>
<th>$\theta$ (degrees)</th>
<th>$T/T_c$</th>
<th>$r_{ret}/\lambda$</th>
<th>$r_{max}/\lambda$</th>
<th>$N_{bun}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Du1</td>
<td>0.00</td>
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<td>0.666667</td>
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Table 5.2: The launching angle $\theta$, period $T$, return and maximum distances, and the bundle number $N_{bun}$, for different values of the crossed-electric-field intensity $f$. The launching azimuth is $\phi = 90^\circ$. Values of $N_{bun}$ become zero when no orbits of that type return within 0.001$\lambda$ of the nucleus.

The important individual orbits, and spectrum of orbits behave as the scaled field is increased. As was the case in the parallel fields and the crossed-fields $\phi = 0^\circ$ cases, a weak electric field only yields a small perturbation in the orbits as seen Table 5.2. Increasing the electric field to a scaled field of $f = 1$, there appear to be no short period orbits which return within 0.001$\lambda$ of the nucleus, and orbits which do appear have quite low stability. Therefore, the oscillations in the spectrum linked to these orbits would be quite weak compared to those depicted for $\phi = 0^\circ$. Figures depicting the orbits detailed in Table 5.2 are presented in Figs. 5.15–5.22.
Figure 5.14: The return distance ($r_{ret}$) against launch polar angle in crossed fields at $\phi = 90^\circ$ and for scaled fields of (a) $f = 0$, (b) $f = 0.001$, (c) $f = 0.1$, and (d) $f = 1$.

Figure 5.15: The coordinate $z$ as a function of the cylindrical coordinate $\rho$ for the orbits evolving from the Garton-Tomkins orbits (“Du1”) as the intensity of the crossed electric field is increased. The electron launches in a vertical plane perpendicular to the electric field direction, i.e., $\phi = 90^\circ$. The panels (a), (b), (c), and (d) are for dimensionless electric-field strength $f = 0, 0.01, 0.1$, and 1, respectively.
Figure 5.16: The $x$-$y$ view of the orbits in Fig. 5.15.

Figure 5.17: As for Fig. 5.15, but for the orbit denoted as “Du2”. Here, like the case for $\phi = 0^\circ$, $\rho$ is now represented as an absolute value due to the different theoretical framework.

Figure 5.18: The $x$-$y$ view of the orbits in Fig. 5.17.

Figure 5.19: As for Fig. 5.17, but for the orbit denoted as “Du3”.

As for Fig. 5.15, but for the orbit denoted as “Du2”. Here, like the case for $\phi = 0^\circ$, $\rho$ is now represented as an absolute value due to the different theoretical framework.
Figure 5.20: The $x$-$y$ view of the orbits in Fig. 5.19.

Figure 5.21: As for Fig. 5.17, but for the orbit denoted as “Du4”.

Figure 5.22: The $x$-$y$ view of the orbits in Fig. 5.21.
In Figs. 5.15 and 5.16, the behaviour of the GT orbit ("Du1") launched perpendicular to an increasing scaled field is depicted. We see, that contrary to the case of $\phi = 0^\circ$ azimuthal launching direction, the orbit expands in size and period with increasing scaled field. Therefore, as the scaled field is increased, the Fourier transformed experimental spectra would expect to see a broadening of peaks as orbit periods are dependant on azimuthal launch angle. We may also expect this broadened peak to have two maxima at the periods associated with orbits shown in Fig. 5.4, as those orbits pass much closer to the nucleus than those presented here.

Figures 5.17 and 5.18 show the behaviour of the orbit denoted as “Du2” as the scaled field is increased for an azimuthal launch angle perpendicular to the applied electric field. This orbit shows much the same behaviour as the GT orbit with the size, and therefore period increasing with increasing scaled field. The behaviour of the polar launch angle is also the same as for the $\phi = 0^\circ$ case in that launch angles are slowly shifting towards the plane perpendicular to the applied magnetic field with increasing scaled field.

The behaviour of the orbit denoted as “Du3” is shown in Figs. 5.19 and 5.20 for the case of perpendicular azimuthal launch angle. This orbit, for the most part, follows the same behaviour as outlined for “Du2”. However, at the high scaled field of $f = 1$, the polar launch angle deviates from the expected behaviour and shifts towards the magnetic field direction rather than the electric field.

Figures 5.21 and 5.22 show the behaviour of the orbit denoted as “Du4” for the case of perpendicular azimuthal launch angle with respect to the applied electric field. This particular orbits behaviour is quite different to that of those discussed previously. While this orbit does expand with increasing scaled field, the period between $f = 0$–0.1 decreases, before increasing again at high scaled field. The polar launch angle also shows contrary behaviour at weak fields with the launch angle increasing, and then decreasing again at high scaled fields.

We would like to stress here that at high scaled fields, all of the orbits discussed above fail to return within 0.001\(\lambda\) of the nucleus, and are therefore not classified as closed orbits. Therefore, effects from these orbits would be minimal in experimental measurements. There is only one orbit at high scaled field which shows significant stability ($N_{\text{bun}} = 862$). This orbit is shown in Fig. 5.23.
5.3.2 Varying scaled energy for specific azimuthal launch angles

In this section, rather than analysing how the spectrum of orbits and individual orbits evolve with varying the scaled field as in Sec. 5.3.1, we look to investigate the effect of varying the scaled energy over the range that has been found to be applicable in the specific case of silicon in Chap 2. As was the case for parallel fields in Sec. 4.3.2, we will focus on the high field regime at \( f = 1 \), and vary the scaled energy over the range \( E_c = 0–4 \) in integer steps to observe how both the entire spectrum of orbits, and the individual orbits themselves vary over this range.

We start by focussing on the \( \phi = 0^\circ \) azimuthal plane. Figure 5.24 shows the spectrum of orbits as the scaled energy is increased in integer steps. As was seen in Sec. 5.3.1, the orbits which are the most stable at \( f = 0 \) (“Du1”–“Du4”) are no longer the dominant orbits at \( f = 1 \). Therefore, instead of tracking those particular orbits in this section (those orbits are presented in Appendix B for every scaled field and scaled energy value considered in this chapter), we will instead give the details of the four most stable closed orbits of the system. In some cases, less than four stable orbits exist for a given scaled energy, in such cases all closed orbits identified will be presented. Table 5.3 gives the characteristics of the four most stable orbits at a high scaled field of \( f = 1 \) and positive integer values of the scaled energy between \( E_c = 0–4 \). Figures 5.25–5.33 show the orbits listed in Table 5.3.
<table>
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<th>$T/T_c$</th>
<th>$r_{\text{ret}}/\lambda$</th>
<th>$r_{\text{max}}/\lambda$</th>
<th>$N_{\text{bun}}$</th>
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Table 5.3: The launching angle $\theta$, period $T$, return and maximum distances, and the bundle number $N_{\text{bun}}$, for different values of the scaled energy $\mathcal{E}_c$ for a fixed value of the crossed scaled electric field $f = 1$. The four most stable orbits at each scaled field and energy combination are given. The launching azimuth is $\phi = 0^\circ$. The orbit index numbers are listed as the most stable, to least stable orbit at those particularly scaled energy values unless otherwise labelled to correspond to orbits previously investigated. The orbit index numbers are not linked, in this instance, between different scaled energy values and may represent totally different orbits.
CHAPTER 5. CROSSED EXTERNAL FIELDS

Figure 5.24: The return distance \( r_{\text{ret}} \) against launch polar angle in crossed fields at \( \phi = 0^\circ \) and for scaled energy of (a) \( \mathcal{E}_c = 0 \), (b) \( \mathcal{E}_c = 1 \), (c) \( \mathcal{E}_c = 2 \), (d) \( \mathcal{E}_c = 3 \), and (e) \( \mathcal{E}_c = 4 \) at a fixed scaled field of \( f = 1 \). Panel (e) is zoomed in an extra two orders of magnitude to reveal the only closed orbit of the system at \( \mathcal{E}_c = 4 \) and \( f = 1 \).


**Figure 5.25:** The coordinate $z$ as a function of the cylindrical coordinate $\rho$ for four most stable orbits at scaled energy $\mathcal{E}_c = 0$ for a scaled field of $f = 1$. The electron launches in a vertical plane containing the electric field direction, i.e., $\phi = 0^\circ$. The panels (a), (b), (c), and (d) are for orbits denoted 1, 2, “Du3”, and 4 respectively from Table 5.3.

**Figure 5.26:** The $x$-$y$ view of the orbits in Fig. 5.25.

**Figure 5.27:** As for Fig. 5.25 but for $\mathcal{E}_c = 1$.

**Figure 5.28:** The $x$-$y$ view of the orbits in Fig. 5.27.
CHAPTER 5. CROSSED EXTERNAL FIELDS

Figure 5.29: As for Fig. 5.25 but for $E_c = 2$.

Figure 5.30: The $x$-$y$ view of the orbits in Fig. 5.29.

Figure 5.31: As for Fig. 5.25 but for $E_c = 3$.

Figure 5.32: The $x$-$y$ view of the orbits in Fig. 5.31.
Figures 5.25 and 5.26 show the four most stable closed orbits at $f = 1$ and $E_c = 0$. The two most stable orbits are the fourth and seventh harmonics of the GT orbit as displayed in panels (a) and (b) respectively. The third most stable orbit is the orbit denoted as “Du3” which is shown in panel (c) of both figures and identified earlier in Sec. 5.3.1. The fourth most stable orbit shown in panel (d) of both figures is a new orbit which was not identified as being one of the most stable orbits at low scaled fields. Analysing the orbit closer, the shape of the orbit before the first pass close to the nucleus (red to green) resembles the shape of the orbit denoted as “Du4” in earlier investigations. The orbit then continues with the final section (blue) resembling the orbit denoted as “Du2” in earlier investigations. Therefore this orbit can be considered as a composite, and closely related to both of these more prominent orbits at low scaled field.

Figures 5.27 and 5.28 show the four most stable closed orbits at $f = 1$ and $E_c = 1$. Panel (a) in both figures show that, at this scaled field and energy value, the orbit denoted at “Du4” is the most stable closed orbit. Panel (b) in both figures show the second most stable orbit which is a new orbit related closely to the orbit denoted as “Du3” in previous investigations. This particular orbit is also described by Du et al. in Fig. 8 of Ref. [2] as being the thirteenth most stable orbit at $f = 0$ and $E_c = 0$. Panel (c) in both figures show the third most stable orbit as being another orbit not previously observed as being particularly stable at low scaled fields. Panel (d) of both figures show the fourth most stable orbit which is again a new orbit. Inspecting of the shape of this orbit closer, it appears once again to be a composite of orbits closely related to the more familiar orbits denoted as “Du3” and “Du4” in earlier investigations.

Figures 5.29 and 5.30 show all of the closed orbits that exist at $f = 1$ and $E_c = 2$. All three orbits are new orbits which have not appeared as particularly stable at
low scaled fields. The orbit shown in panel (a) of both figures appears to be closely related to the orbit denoted as “Du4” in earlier investigations. The other two orbits in panels (b) and (c) do not appear to be closely related to orbits which have been investigated in previous sections. However, given their bundle numbers from Table 5.3 are $N_{\text{bun}} = 4$ and $N_{\text{bun}} = 3$ respectively, neither of these orbits are particularly stable and would not contribute to experimental data.

Figures 5.31 and 5.32 show the four most stable closed orbits at $f = 1$ and $E_c = 3$. As at $E_c = 2$, all of the closed orbits here have not been identified previously in other investigations. The orbits in panels (a) and (b) of both figures are closely related to the orbit denoted as “Du4” in previous investigations. The orbits displayed in panels (c) and (d) of both figures do not appear to be related to orbits discussed in previous sections despite the orbit in panel (c) having a nearly identical projection in the $x-y$ plane to the orbits shown in panels (a) and (b).

At $f = 1$ and $E_c = 4$, as shown in Fig.5.33, only one stable closed orbit exists in the form of the fourth harmonic of the GT orbit (“Du1”).

Moving on to the $\phi = 90^\circ$ azimuthal plane, Fig.5.34 shows the spectrum of orbits as the scaled energy is increased in integer steps. As was the case for the $\phi = 0^\circ$ azimuthal plane, we look to investigate the four most stable orbits at each value of the scaled energy. Table 5.4 gives the characteristics of the four most stable orbits at $f = 1$ and for each integer value of the scaled energy between $E_c = 0–4$. Figures 5.35–5.42 show the orbits listed in Table 5.4.
Figure 5.34: The return distance ($r_{ret}$) against launch polar angle in crossed fields at $\phi = 90^\circ$ and for scaled energy of (a) $\mathcal{E}_c = 0$, (b) $\mathcal{E}_c = 1$, (c) $\mathcal{E}_c = 3$, and (d) $\mathcal{E}_c = 4$ at a fixed scaled field of $f = 1$. The figure at $\mathcal{E}_c = 2$ is omitted due to there being no stable closed orbits at that particular energy.
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<td>Du4</td>
<td>80.470</td>
<td>2.85057</td>
<td>$3.37 \times 10^{-4}$</td>
<td>1.06652</td>
<td>26</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>79.967</td>
<td>3.80807</td>
<td>$1.19 \times 10^{-4}$</td>
<td>1.06866</td>
<td>6</td>
</tr>
</tbody>
</table>

Table 5.4: The launching angle $\theta$, period $T$, return and maximum distances, and the bundle number $N_{\text{bun}}$, for different values of the scaled energy $\mathcal{E}_c$ for a fixed value of the crossed scaled electric field $f = 1$. The four most stable orbits at each scaled field and energy combination are given. The orbit index numbers are as the most stable, to least stable orbit at those particularly scaled energy values unless otherwise labelled to correspond to orbits previously investigated. The orbit index numbers are not linked in this instance between different scaled energy values and may represent totally different orbits.
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Figure 5.35: The coordinate $z$ as a function of the cylindrical coordinate $\rho$ for four most stable orbits at scaled energy $\mathcal{E}_c = 0$ for a scaled field of $f = 1$. The electron launches in a vertical plane perpendicular to the electric field direction, i.e., $\phi = 90^\circ$. The panels (a), (b), (c), and (d) are for orbits denoted 1, 2, 3, and 4 respectively from Table 5.4.

Figure 5.36: The $x$ - $y$ view of the orbits in Fig. 5.35.
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Figure 5.37: As for Fig. 5.35 but for $\mathcal{E}_c = 1$.

Figure 5.38: The $x$-$y$ view of the orbits in Fig. 5.37.

Figure 5.39: As for Fig. 5.35 but for $\mathcal{E}_c = 3$.

Figure 5.40: The $x$-$y$ view of the orbits in Fig. 5.39.
Figures 5.35 and 5.35 show the four most stable closed orbits at $f = 1$ and $\mathcal{E}_c = 0$. Panel (a) in both figures shows the most stable orbit which is related to the orbit denoted as “Du4” in previous investigations, except that it has an extra loop on positive z-axis side. Panel (b) in both figures shows the second most stable orbit. Here, the first part of the orbit (red to green) follows a similar path to the orbit denoted as “Du1”. Panels (c) and (d) of both figures show the third and fourth most stable orbits respectively. Neither of these orbits resemble those which are stable at low scaled fields and are considerably more complicated in their structure due to the high electric field.

Figures 5.37 and 5.38 show the four most stable closed orbits for $\mathcal{E}_c = 1$. Panel (a) in both figures show the most stable closed orbit, which is another new orbit not closely linked to the more stable closed orbits at low scaled field. Panel (b) in both figures show the second most stable closed orbit which shares the same shape as the corresponding panels at $\mathcal{E}_c = 0$. Whilst the orbits have the same shape, the increase in scaled energy has lead to this orbit becoming less stable as noted by the corresponding bundle numbers in Table 5.4. Panels (c) and (d), as in the $\mathcal{E}_c = 0$...
case, show orbits which do not resemble any of the most stable closed orbits at low scaled field.

Figures 5.39 and 5.40 show the four most stable closed orbits at $E_c = 3$. At this particular scaled energy, the orbit denoted as “Du2” in previous investigations is the most stable closed orbit of the system as shown in panel (a) of both figures. The second most orbit, as shown in panel (b) of both figures, is an orbit closely related to the orbit denoted as “Du4” in previous investigations, except that it has an extra loop on the negative $z$-axis side of the orbit. The third most stable orbit, shown in panel (c) of both figures, is another new orbit which is not closely linked to any of the most stable orbits at low scaled field. The fourth most stable orbit is an interesting combination of the orbits denoted as “Du2” and “Du3” in previous investigations. Other composite orbits which have been discussed in this section have the first orbit traversed completely, but not classified as closed, before moving off from close to the nucleus to complete the second orbit. Here, only the first half of the orbit denoted as “Du2” is completed before breaking off into the orbit shape identified as “Du3” before coming back to finish the final half of the “Du2” shape. Therefore, rather than having two close passes to the nucleus which break the orbit into two separate shapes, this particular orbit only has one close pass to the nucleus.

Figures 5.41 and 5.42 show the four most stable closed orbits of the system at a scaled energy of $E_c = 4$. Interestingly, the three most stable orbits of the system under these conditions are those denoted as “Du1”, “Du2”, and “Du4” respectively from previous investigations. The fourth most stable orbit is interesting in that it is a composite of the same orbit, which is denoted as “Du2” in previous investigations. This orbit also closely resembles the fourth most stable orbit at $E_c = 3$, in that only the first half of the positive $z$-axis “Du2” orbit is traversed before following a trajectory associated with the negative $z$-axis “Du2” orbit, which returns to then finish the second half of the positive $z$-axis “Du2” orbit.
5.3.3 Azimuthal dependence of Garton-Tomkins orbit

In this section, we focus solely on the GT orbit, which is known to be the most important orbit in the analysis of experimental spectra in the crossed-fields geometry [44]. For any value of the scaled field, or scaled energy, the GT orbit has a polar launch angle of $\theta = 90^\circ$ relative to the applied magnetic field. In the case of silicon, this is only true in the case of the magnetic field being aligned along a conduction band valley. As was discovered in Chap. 3, if the magnetic field is aligned in any other direction, the GT orbit is pulled out of the perpendicular plane due to the anisotropy of the system.

Under the conditions of a closed orbit needing to return within $0.01\lambda$ in less than $5T_c$, the GT orbit has seven harmonics which return to the nucleus for $f = \mathcal{E}_c = 0$ which are shown in Fig. 5.43. Different harmonics were defined by the number of local minima present in the orbit trajectory with reference to the nucleus. At low scaled fields and energies this is trivial; however, at high scaled fields and energies, the orbits become much more complicated and identification of different harmonics becomes increasingly difficult.

The azimuthal launch angle was sampled at $\Delta \phi = 0.1^\circ$ intervals, and return angles were calculated as the electron azimuth at the twentieth last sample point of a given loop of its trajectory. This choice is due to the majority of orbits in this

Figure 5.43: The seven harmonics of the GT orbit for $f = \mathcal{E}_c = 0$ and $\phi = 0^\circ$. The colour of the orbit evolves with time from launch (red) to return (blue) as denoted by the direction of the arrows. The beginning of the orbit is not visible after the third harmonic due to the overlap as it undergoes a greater than $360^\circ$ rotation about the $z$-axis. The periods of these harmonics are successive multiples of $2T_c/3$. 
system, at finite scaled fields and energies, not being completely closed. Therefore, the closest point to the nucleus may lie in a different angular region to the general return direction of the orbit. We found, through analysing orbits whose curvature was high around the nucleus, that the omission of the final nineteen points was sufficient to minimize this effect as seen in Fig. 5.44. The return angles should therefore be seen as good approximates, rather than exact quantities, and are more accurate for orbits who return closest to the nucleus. Panels (a), (b), and (c) of Fig. 5.44 show an example of this phenomenon where the final point would yield a return angle of $\phi \sim 315^\circ$ rather than the $\sim 120^\circ$ expected.

**Figure 5.44:** Panels (a), (b), and (c) show an example of a seemingly closed orbit for $f = 0.01$, $E_c = 0$, and $\phi = 0^\circ$. Panel (a) is the entire orbit, panel (b) zooms in on the region around the nucleus to reveal the problem with using the closest point for calculating the return angle. Panel (c) shows the orbit minus the last nineteen points to reveal a good estimate of the return angle. Note panel (b) is magnified two orders of magnitude further than panel (c). Panel (d) shows the calculated return angle as a function of the number of data points omitted from the closest pass to the nucleus. Two orbits of high curvature near the nucleus from Fig. 5.51 were considered. After $\sim 20$ points from the nucleus, the return angle stabilizes and was therefore utilised as our condition for the calculation of the return angle.
5.3.3.1 Scaled field dependence of launch and return angles

In this section, we systematically increase the scaled field, at a fixed scaled energy of $E_c = 0$, to investigate how the azimuthal dependencies of the first seven harmonics of the GT orbit evolve in crossed magnetic and electric fields.

We first consider the case of magnetic-field alone. Figure 5.45 shows the azimuthal dependence of both launch and return angles for the GT orbit and its harmonics under pure magnetic-field conditions ($f = 0$). There is no azimuthal angle dependence in this case, as expected, given the rotational symmetry of the system in a pure magnetic field. The variation in return distance for the different harmonics is an artefact of the numerical procedure rather than a real physical effect. However, considering the scale of the left axis, all harmonics return very close to the nucleus and in the following numerical results hereafter, this effect is negligible as the scale increases.

We now introduce a small electric field along the $x$-axis perpendicular to the applied magnetic field. Figure 5.46 shows the azimuthal dependence of both launch and return angles of the GT orbit with a small crossed electric field of $f = 0.01$ applied in the plane perpendicular to the magnetic field along $\phi = 0^\circ$. This small perturbation is enough to break the rotational symmetry of the system and a two-fold azimuthal dependence appears in both launch and return angles, corresponding to orbits returning with or against the electric field. This is in accordance to what was...
Figure 5.46: Return distance ($r_{\text{ret}}$) to the nucleus as a function of azimuthal (a) launch and (b) return angle for $f = 0.01$ and $E_c = 0$.

observed in bound closed orbits [45] and what was observed earlier in this chapter in Fig. 5.4. Interestingly, the third and sixth harmonics show no azimuthal dependence. Intuitively, one would expect these harmonics to show at least some azimuthal dependence, especially given their periods are longer than the first a second harmonics. These azimuthal-angle independent harmonics are essentially periodic and have a three-fold rotational symmetry about the $z$-axis as shown in Fig. 5.43, therefore, the net effect of the electric field along them is negligible.

From the scale on the left side of Fig. 5.46, which is of the order of $10^{-6}\lambda$, we can see that the azimuthal angle dependence is relatively weak as the entire 360° range contains closed orbits. Interestingly, the return distance for the azimuthal-dependent harmonics is nearly identical for different harmonics of similar return angle in Fig. 5.43. In regards to the minima of the return angle of the azimuthal-dependent harmonics, the closest pass to the nucleus occur at azimuthal angles which fall away from the angles at $\phi = 0^\circ$, $90^\circ$, $180^\circ$, and $270^\circ$, on the plane perpendicular to the magnetic field. One may then expect the azimuthally-independent harmonics to contribute the strongest oscillations to the spectrum. However, this would be a false conclusion, given that the lower harmonics have a much stronger stability under variation of the polar launch angle. This can be observed in Fig. 2.3 (b) with increasing sharpness of the parabolic dispersion for the GT orbit as the harmonic number increases.

Whilst not studied in detail within this work, recurrence strengths observed from closed orbits in atomic systems, and those in an anisotropic environment such as silicon, may differ due to the presence of six conduction-band valleys. In atomic systems for the case of $f = 0$, the recurrence peak heights decrease with increasing
harmonics due to their corresponding polar angle dependencies.

The azimuthal dependence observed in non-rotationally-symmetric orbits gives an insight into resonances in the crossed-field geometry being weaker than those in rotationally-symmetric systems [23, 47]. In such cases, every closed orbit is part of an essentially infinite family of closed orbits sharing the same polar launch angle but different azimuthal launch angles. In the crossed-fields case, due to the loss of rotational symmetry, this is no longer the case, as is seen in the azimuthal dependencies obtained in the calculations.

We now increase the electric field further. Figure 5.47 shows the azimuthal angle dependence of launch and return angles with the scaled field raised by an order of magnitude to \( f = 0.1 \). The azimuthal-dependent harmonics from Fig. 5.46 show

\[ f = 0.1, \mathcal{E}_c = 0 \]

\[ f = 0.1, \mathcal{E}_c = 0 \]

\[ f = 0.1, \mathcal{E}_c = 0 \]

\[ f = 0.1, \mathcal{E}_c = 0 \]

Figure 5.47: Return distance \((r_{\text{ret}})\) to the nucleus as a function of azimuthal launch (left column) and return (right column) angle for \( f = 0.1 \) and \( \mathcal{E}_c = 0 \). The second row is a magnification of the first row to reveal the relatively weak azimuthal angle dependencies of the third and sixth harmonics virtually the same two-fold launch and return azimuthal angle dependence as before, except now on a much larger scale of \( 10^{-4}\lambda \). Interestingly, with the increase in
scaled field leading to a stronger perturbation away from the rotational symmetry at zero field, the peaks alternate between shortest and longest harmonics returning closer to the nucleus. The azimuthal-independent harmonics from Fig. 5.46 appear to continue showing no azimuthal dependence until we zoom in to reveal a very small four-fold launch and return azimuthal dependence in Figs. 5.47 (c) and (d). We attribute this four-fold azimuthal dependence to these orbits having an approximate rotational symmetry about the $z$-axis. The field has perturbed these harmonics enough from this rotational symmetry that every pass of either the $x$ or $y$-axis yields a shift from being predominately with or against the electric field, leading to the four-fold azimuthal angle dependence observed. In the first, fourth, and seventh harmonics, the minima around $\phi = 45^\circ$ in return angle have become slightly more stable relative to the minima around $\phi = 225^\circ$. To be concrete, an orbit is more stable than another if it has a higher number of neighbouring orbits which are considered as closed orbits. The number of neighbouring orbits is, of course, dependent on the sampling step size of the calculations, as realistically, there is a continuous spectrum if orbits which can not be enumerated. However, for a constant step size in azimuthal angle, an increase in stability is identified as a widening of the parabolic dispersion at $\phi = 45^\circ$ return angle relative to the dispersion centred at $\phi = 225^\circ$. A similar behaviour is also observed for the second and fifth harmonics. It is interesting to note that the launch and return angles of the third and sixth harmonics in Figs. 5.47 (c) and (d) occur near the angles $\phi = 0^\circ$, $90^\circ$, $180^\circ$ and $270^\circ$ with respect to the external-electric-field orientation. We expect this to lead to different relative peak heights in experimental results between these harmonics and the others than observed at $f = 0$.

Increasing the scaled field further, Fig. 5.48 shows the azimuthal angle dependence of launch and return angles for a scaled field of $f = 0.25$. The azimuthal dependencies have grown so much that there are angles where the azimuthal-dependent harmonics of Fig. 5.46 are no longer considered as containing closed orbits. The relative stability of the third harmonic, especially, is still very strong, as indicated by its small azimuthal dependence. The increase in scaled field leads to some minima positions beginning to shift. Specifically, for the azimuthal-dependent harmonics in Fig. 5.46, the longer-period harmonics shift their minima away from the minima of the shorter-period harmonics and towards the electric-field orientation. A different effect is observed in the third and sixth harmonics, with the latter shifting the two minima at $\phi = 0^\circ$ and $\phi = 180^\circ$ away from the minima shared with the third harmonic at lower fields. However, the other two minima at $\phi = 90^\circ$ and $\phi = 270^\circ$ remain tied to the third harmonic. The increase in stability of return-angle minima in the $\phi = 0–180^\circ$ range over minima in the $\phi = 180–360^\circ$ range has also become
more pronounced with the increase in scaled field.

Figures 5.49 (a) and (b) show the azimuthal angle dependence of launch and return angles for a scaled field of $f = 0.5$. The electric-field strength has perturbed the system to the extent that harmonics previously seen as weakly azimuthally dependent now show a strong azimuthal dependence, leading to a more complicated picture of the system. Due to the complicated nature of these figures, and subsequent figures at higher scaled fields, it is more useful to separate harmonics who shared the same return angle at zero scaled field into different figures to allow an easier analysis of the system. These are shown in Figs. 5.49 (c) – (h).

Panels (c) and (d) from Fig. 5.49 show the launch and return azimuthal dependencies of the first, fourth, and seventh harmonics. The longer-period harmonics become increasingly separated from the first harmonic as the scaled field is increased and the minima of the seventh harmonic is now closest to the electric-field orientation. The difference in stability between the two minima of the same harmonic is also further accentuated with the seventh harmonic showing a significant increase in stability over the shorter-period harmonics.
Figure 5.49: Return distance ($r_{\text{ret}}$) to the nucleus as a function of azimuthal (a) launch and (b) return angle for $f = 0.5$ and $\mathcal{E}_c = 0$. Due to the complexity of (a) and (b), further panels are given for harmonics who have the same return angle at low scaled fields to gain a better insight into the evolution of the system. The second row shows the first, fourth, and seventh harmonics, the third row shows the second and fifth harmonics, and the fourth row shows the third and sixth harmonics.
In panels (e) and (f) of Fig. 5.49 the second and fifth harmonics are shown. The opposite behaviour is observed in these harmonics than was observed for the first, fourth, and seventh harmonics with the fifth harmonic being drawn away from the electric-field orientation. As seen for the seventh harmonic, as the fifth harmonic is being drawn away from the second harmonic by the increasing electric field, the stability increases.

Panels (g) and (h) of Fig. 5.49 show the third and sixth harmonics which, at low fields, showed no azimuthal dependence. Here, the sixth harmonic shows the strongest azimuthal dependence, as one would expect, given its longer orbit period. These harmonics minima positions have diverged from each other around $\phi = 0$ and $180^\circ$, however, remain more closely tied together at $\phi = 90$ and $270^\circ$.

Doubling the field now, Fig. 5.50 shows the azimuthal angle dependence of launch and return angles for both the entire set of harmonics, and selected harmonics, at $f = 1$. Here the complexity of the results has increased and harmonics sharing the same return angle at zero scaled field need to again be considered separately. At this high scaled field, the relationship between comparable harmonics has been essentially broken. This can be seen most readily in panels (c) and (d) of Fig. 5.50, where there is no longer a resemblance between harmonics previously observed to be similar in nature. The first harmonic here remains relatively unchanged from earlier figures, however, the fourth and seventh harmonics have broken their two-fold symmetry with new minima presenting themselves in the results. There is a discontinuity in the calculations due to orbits breaking the $5T_c$ threshold. A new kind of feature presents itself in the fourth harmonic between $\phi = 200$ and $250^\circ$ launch angle and $\phi = 90$ and $135^\circ$ return angle. In return angle, rather than the standard parabolic dispersion in return distance with azimuthal angle, the curve folds back, almost upon itself, once reaching the minimum. In Fig. 5.51 a series of fourth harmonic orbits with increasing launch angle in this region show this is not an artefact of the return-angle calculation process, but rather a real effect due to the relative strength of the electric field.
Figure 5.50: Return distance \( r_{\text{ret}} \) to the nucleus as a function of azimuthal (left column) and return (right column) angle for entire set of harmonics and comparable harmonics at \( f = 1 \) and \( E_c = 0 \)
Figure 5.51: Variation of the fourth harmonic as the launch angle (denoted as “L” in figure titles) is increased from $\phi = 200^\circ$ to $250^\circ$ in $5^\circ$ increments. The colour of the orbit evolves with time from launch (red) to return (blue) as denoted by the direction of the arrows. The return angle (denoted as “R” in figure titles) increases with launch angle until $\phi = 225^\circ$, after which it decreases with increasing launch angle leading to the unusual feature present in Fig. 5.50 (d).
Panels (e) and (f) of Fig. 5.50 show the second and fifth harmonics, where large angular regions of essentially closed orbits now dominate the azimuthal spectrum. This resembles the “orbit mixing” observed in Sec. 4.3.3 in Chap. 4 and is characteristic of a bifurcation process which leads to the breaking of previous held azimuthal symmetries. A finer mesh of scaled fields in the region from \( f = 0.5 - 1 \) (presented in Sec. 5.3.3.3) shows these large angular regions were also present before the breaking of symmetries in the fourth and seventh harmonics in panels (c) and (d) of Fig. 5.50. These bifurcations may be experimentally observable, as bifurcation processes have been in other field configurations in atomic systems [21, 37, 39, 45, 50, 62]. Furthermore, the scaled fields at which this is being observed in the crossed-fields system are similar to those found for the parallel-fields geometry in Chap. 4.

Conversely to the other harmonics, panels (g) and (h) of Fig. 5.50 show the third and sixth harmonics retaining their four-fold symmetry. However, their minima have shifted away from their low-field positions completely. Perhaps surprisingly, minima which were shared between these harmonics at lower scaled fields are still present even at this high scaled field.

Increasing the field further, Fig. 5.52 shows the azimuthal angle dependence of launch and return angles for both the entire system, and selected harmonics, at \( f = 1.5 \). As at \( f = 1 \), the system is very complicated and harmonics sharing the same return angle at zero scaled field need to be considered separately. Concentrating on the first, fourth, and seventh harmonics in panels (c) and (d) of Fig. 5.52, the fourth harmonic is showing an increased stability as it aligns itself with the external electric field. Given we have moved from low to high scaled fields, the first harmonic has remained relatively unchanged, in that it has retained its two-fold azimuthal dependence and its minima remain close to their original positions at low scaled field.

In the second and fifth harmonics shown in panels (e) and (f) of Fig. 5.52, the fifth harmonic still presents a large area of stability in the return angle. The second harmonic now shows a clear four-fold azimuthal dependence at this high scaled field due to the bifurcation seen occurring at \( f = 1 \). The fifth harmonic shows a much higher degree of azimuthal dependence indicating it has undergone many bifurcations.

In panels (g) and (h) of Fig. 5.52, the third and sixth harmonics, which up until \( f = 1 \) had held their original four-fold symmetry, now display six-fold and eight-fold azimuthal dependencies respectively, indicating they have undergone many bifurca-
Over the course of Sec. 5.3.3.1, we have shown the return distance as a function of both launch and return angle separately. While this is insightful for investigating the azimuthal dependencies of the harmonics, the relationship between launch and return angles is difficult to access. In Fig. 5.53, we show the return angle as a function of launch angle as the scaled field is increased from $f = 0 - 1.5$. As is expected at $f = 0$, due to the rotational symmetry of the system, there is a linear relationship between launch and return angles. However, as the scaled field is increased, and the rotational symmetry is broken, the linear relationship between launch and return angles is also broken. Discontinuities begin to appear in the curves at $f = 0.25$ due to orbits not returning within 0.001$\lambda$ of the nucleus. Moving to higher scaled fields, the gradients of the lines vary substantially. A steep gradient would indicate greater chaos in the orbit, as a small change in initial launch angle results in a large variation in return angle. Conversely, a shallow gradient would indicate an element of stability in the orbits, as a small variation in return angle is observed for large variations in initial launch angle. Interestingly, at high scaled fields, the closed orbits seem to congregate along the diagonals of the figures. Orbits which arrange themselves along the diagonal defined by equal launch and return angles correspond to orbits with high rotational symmetry about the magnetic field, which we have shown to be more stable to variations in scaled field in earlier figures.
Figure 5.52: Return distance ($r_{ret}$) to the nucleus as a function of azimuthal (left column) and return (right column) angle for entire set of harmonics and comparable harmonics at $f = 1.5$ and $E_c = 0$. 
Figure 5.53: Return angle as a function of launch angle for $f = 0 - 1.5$ and $E_c = 0$
5.3.3.2 Scaled energy dependence of launch and return angles

In this section, we focus on fixing the scaled field and varying the scaled energy. The purpose is to investigate how increasing the scaled energy affects the symmetries of the first seven harmonics of the GT orbit. The scaled energy is varied in integer steps over the region $E_c = 0–4$. This region of scaled energy was shown in Chap. 2 to be important in the analysis of experimental results published in silicon [19]. The scaled field is taken at fixed values of $f = 0.25$ and 0.5, as these scaled fields showed interesting features in the calculations.

Figures 5.54 and 5.55 show the launch and return azimuthal dependencies for the seven harmonics of the GT orbit as the scaled energy is incrementally increased for a fixed scaled field of $f = 0.25$. As has been shown in previous chapters, increasing the scaled energy in such a way affects the periods of the orbits substantially. This can be observed in these figures as changes in shading as the scaled energy is increased. The sixth and seventh harmonics disappear from the calculations altogether at $E_c = 3$ and $E_c = 1$ respectively, as they now exceed $5T_c$. The first and fourth harmonics are shown on the left columns of these figures. The first harmonic showed very little change when increasing the scaled field in Sec. 5.3.3.1, however, with increasing scaled energy, the launch and return angle minima are shifting towards $\phi = 90$ and $270^\circ$. This effect is not observed in Sec. 5.3.3.1 and points to the scaled energy being a more effective tool in shifting the minima of these orbits with respect to the external electric-field orientation.

The fourth harmonic undergoes another form of bifurcation with increasing scaled energy between $E_c = 2$ and $E_c = 4$, moving from a two-fold to four-fold azimuthal dependence. At $E_c = 3$, a large azimuthal region of essentially closed orbits exists which is an indication of a bifurcation process taking place. One would expect this feature to cause an increase in experimental recurrence peak height at this scaled energy for this harmonic. Therefore, in the crossed-fields system, bifurcations occur either with varying scaled field or scaled energy.
Figure 5.54: Return distance ($r_{rel}$) to the nucleus as a function of azimuthal launch angle at $f = 0.25$ as the scaled energy is increased in integer increments from $E_c = 0$ to 4. In the figure, scaled energy increases from top to bottom. The left column shows the first, fourth, and seventh harmonics, the middle column, the second and fifth harmonics, and the right column, the third and sixth harmonics.
Figure 5.55: Return distance ($r_{\text{rel}}$) to the nucleus as a function of azimuthal return angle at $f = 0.25$ as the scaled energy is increased in integer increments from $\mathcal{E}_c = 0$ to 4. In the figure, scaled energy increases from top to bottom. The left column shows the first, fourth, and seventh harmonics, the middle column, the second and fifth harmonics, and the right column, the third and sixth harmonics.
The middle columns of Figs. 5.54 and 5.55 show the second and fifth harmonics evolution with increasing scaled energy. In this scaled energy range, both harmonics undergo bifurcations and move from two-fold to four-fold azimuthal dependencies. The fifth harmonic having the longest period, is more susceptible to changes in the system. Therefore, its bifurcation process occurs at a lower value of $E_c = 1$ than the second harmonics’ at $E_c = 3$. The fifth harmonic also shows the potential for another bifurcation at scaled energy exceeding $E_c = 4$. Both bifurcations in the two harmonics occur over large launch and return azimuthal angle regions, and therefore will have a significant affect in experimental data.

The right columns in Figs. 5.54 and 5.55 show the third and sixth harmonics and their evolution with increasing scaled energy. Interestingly, these harmonics undergo a bifurcation between $E_c = 0$–1, however, they move from a four-fold azimuthal dependence back to two-fold. This seems at odds with every other bifurcation process observed, as they all move from a lower to higher azimuthal angle dependence. This different form of bifurcation is examined in more detail in Sec. 5.3.3.4.

Figures 5.56 and 5.57 show the launch and return azimuthal dependencies for the seven harmonics of the GT orbit as scaled energy is incrementally increased for a fixed scaled field of $f = 0.5$. The first harmonic shows the same behaviour as was observed at $f = 0.25$ with the launch and return angle minima moving towards $\phi = 90^\circ$ and $\phi = 270^\circ$ with increasing scaled energy. The fourth harmonic once again undergoes a bifurcation moving from a two-fold to four-fold dependence. However, here the bifurcation appears at a lower scaled energy than previously seen at $f = 0.25$ due to the instability the higher scaled field induces in the azimuthal dependence. This bifurcation also evolves in the same way be seen when comparing figures at $f = 0.25, E_c = 4$ and $f = 0.5, E_c = 2$.

The second harmonic again moves from a two-fold to four-fold dependence through a bifurcation process between $E_c = 1$ and 2. As was the case with the fourth harmonic, the second harmonic undergoes its bifurcation at a lower scaled energy with the increased scaled field. This bifurcation also evolves in the same manner at both scaled fields. The fifth harmonic starts starts as a two-fold dependence at $E_c = 0$ and undergoes many bifurcations and azimuthal-dependence symmetries with increasing scaled energy. The major bifurcation occurs between $E_c = 0$ and 1. As was the case with other harmonics discussed, this bifurcation occurs at lower scaled energy than was observed at $f = 0.25$. 

FIGURE 5.56: Return distance ($r_{\text{ret}}$) to the nucleus as a function of azimuthal launch angle at $f = 0.5$ as the scaled energy is increased in integer increments from $E_c = 0$ to 4. In the figure, scaled energy increases from top to bottom. The left column shows the first, fourth, and seventh harmonics, the middle column, the second and fifth harmonics, and the right column, the third and sixth harmonics.
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Figure 5.57: Return distance ($r_{\text{ret}}$) to the nucleus as a function of azimuthal return angle at $f = 0.5$ as the scaled energy is increased in integer increments from $\xi_e = 0$ to 4. In the figure, scaled energy increases from top to bottom. The left column shows the first, fourth, and seventh harmonics, the middle column, the second and fifth harmonics, and the right column, the third and sixth harmonics.
The third and sixth harmonics, in contrast to those discussed previously, have a much different azimuthal dependence than was observed at $f = 0.25$. The shift from four-fold to two-fold dependence, seen at $f = 0.25$, no longer occurs. The third harmonic undergoes a new small bifurcation between $E_c = 2$ and $3$ evolving from a four-fold to six-fold azimuthal dependence. The sixth harmonic undergoes a large change between $E_c = 1$ and $2$, with new features presenting themselves in both launch and return angles.

5.3.3.3 Bifurcation evolution with varying scaled field

In Sec. 5.3.3.1, numerous bifurcations and changes in symmetry were visible in calculations when increasing the scaled field from $f = 0.5$ to $1$. In this section, we focus on this scaled field region in finer detail using increments of $f = 0.05$ to gain a more detailed understanding of the bifurcations and azimuthal dependencies within this range.

Figures 5.58 and 5.59 show the azimuthal angle dependencies of the first, fourth, and seventh harmonics for launch and return angles respectively over this scaled-field range. The first harmonic undergoes very little change in this region. The only noteworthy change coming the orbit returning at approximately $\phi = 250^\circ$ which increases in stability with increased scaled field over this range.

The fourth harmonic also remains relatively unchanged until $f = 0.9$ where a new feature begins to return close enough to the nucleus to be considered as having closed orbits. At $f = 0.95$ this new feature is becoming quite substantial and stable to the point that at $f = 1$, it is the dominant feature in this harmonic. This feature is unusual in that the return-angle azimuthal dependence is non-parabolic in nature. This was explored earlier for this particular case in Fig. 5.51, however, other instances do occur in the calculations for other harmonics and fields.

The seventh harmonic showed significant change in Sec. 5.3.3.1 with a new feature, a discontinuity, and the possibility of a bifurcation in the most stable of the two minima at $f = 0.5$. All of these are now explained in the series of figures shown in this section. The new feature comes about in much the same way as was observed in the fourth harmonic. However, here this feature begins to present itself at $f = 0.6$ and is much more sensitive to variations in scaled field than the regular two-fold dependence. As in the fourth harmonic, this feature presents a non-parabolic relationship in the return-angle azimuthal dependence. At $f = 0.9$, this feature develops a discontinuity, which is due to those missing orbits now exceeding $5T_c$. These orbits would still be present in experimental data of course as this cutoff is arbitrary for
Figure 5.58: Return distance ($r_{\text{ret}}$) to the nucleus as a function of azimuthal launch angle for the first, fourth and seventh harmonics in the scaled-field region of $f = 0.5$ to 1 in steps of $f = 0.05$. 
Figure 5.59: Return distance ($r_{\text{ret}}$) to the nucleus as a function of azimuthal launch angle for the first, fourth and seventh harmonics in the scaled-field region of $f = 0.5$ to 1 in steps of $f = 0.05$. 
numerical purposes. The most stable minima of the two at $f = 0.5$ undergoes its bifurcation from $f = 0.65 - 0.85$ where a significant azimuthal angle range contains essentially closed orbits.

Figures 5.60 and 5.61 show the azimuthal angle dependencies of the second and fifth harmonics for launch and return angles, respectively, over the same scaled-field range. The second harmonic, much like the first, undergoes relatively little change. However, at higher fields, the most stable of the two minima forms a wide range of closed orbits in what looks to be the beginnings of a bifurcation.

The fifth harmonic undergoes a more significant change over this scaled-field range. The most stable minima in this harmonic at $f = 0.5$ continues to increase in stability to the point that at $f = 0.85$, almost a third of the entire azimuthal-angle space is dominated by essentially closed orbits. We should expect such a large feature to be apparent in experimental data. At higher scaled fields this large area undergoes multiple bifurcations, however, the area around $\phi = 180^\circ$ remains very stable in both launch and return angles.

Figures 5.62 and 5.63 show the azimuthal angle dependencies of the third and sixth harmonics for launch and return angles respectively over the same scaled-field range. Both harmonics retain their four-fold azimuthal dependence over this scaled field range. As the scaled field is increased, the orbits in both harmonics become less stable as seen by the increasing curvature of the parabolas in the calculations. The third harmonic begins a small bifurcation process at the higher end of this scaled-field range, however, it is unlikely this would be significant in any experimental results.
Figure 5.60: Return distance ($r_{\text{rel}}$) to the nucleus as a function of azimuthal launch angle for the second and fifth harmonics in the scaled-field region of $f = 0.5$ to 1 in steps of $f = 0.05$. 

![Diagram of Figure 5.60]
Figure 5.61: Return distance ($r_{\text{ret}}$) to the nucleus as a function of azimuthal launch angle for the second and fifth harmonics in the scaled-field region of $f = 0.5$ to 1 in steps of $f = 0.05$. 
Figure 5.62: Return distance ($r_{\text{ret}}$) to the nucleus as a function of azimuthal launch angle for the third and sixth harmonics in the scaled-field region of $f = 0.5$ to 1 in steps of $f = 0.05$. 
Figure 5.63: Return distance ($r_{\text{ret}}$) to the nucleus as a function of azimuthal launch angle for the third and sixth harmonics in the scaled-field region of $f = 0.5$ to 1 in steps of $f = 0.05$. 
5.3.3.4 Reduction of azimuthal dependence in third and sixth harmonics

In Sec. 5.3.3.2, we observed that in Figs. 5.54 and 5.55, the third and sixth harmonics moved from a four-fold to two-fold azimuthal dependence through a bifurcation process when the energy was increased from $E_c = 0$ to $1$. This was unexpected as every other form of azimuthal symmetry change we have observed involved moving from a lower to higher azimuthal angle dependency. In this section, we revisit this feature using a finer scaled energy mesh of $\Delta E_c = 0.1$, to gain a better insight into this different form of bifurcation.

Figures 5.64 and 5.65 show the launch and return azimuthal angle dependencies, respectively, for the third and sixth harmonics at $f = 0.25$ and scaled energies ranging from $E_c = 0$ to $1$ in steps of $0.1$. We observe that as the scaled energy is increased from $E_c = 0$ to $0.1$, the relative height of the peaks in the azimuthal dependence changes substantially. These harmonics appear to be much more sensitive to variations in scaled energy than scaled field. By increasing the scaled energy to $E_c = 0.3$, the two peaks either side of the external electric-field orientation at $\phi = 0^\circ$ have nearly disappeared completely. This creates a large azimuthal area of closed orbits as the scaled energy is incrementally increased, which encompasses the external electric-field orientation at $\phi = 0^\circ$ in both launch and return angles.
Figure 5.64: Return distance ($r_{ret}$) to the nucleus as a function of azimuthal launch angle for the third and sixth harmonics at $f = 0.25$ for varying scaled energy between $E_c = 0$ and 1 in 0.1 steps.
Figure 5.65: Return distance ($r_{ret}$) to the nucleus as a function of azimuthal launch angle for the third and sixth harmonics at $f = 0.25$ for varying scaled energy between $E_c = 0$ and $1$ in $0.1$ steps.
5.4 Conclusion

In this chapter, rather than the external electric and magnetic field being orientated parallel to each other as in Chap. 4, the electric field is applied in the plane perpendicular to the applied magnetic field. This breaks the rotational symmetry and leads to a much more complicated system to study classically. In Sec. 5.2, we develop a new simplified theoretical framework for the investigation of this problem classically. The relative simplicity of this theory, compared to the Kustaanheimo-Stiefel transformation, allows the calculation of classical orbits in a less numerically intensive manner. Moving to the numerical analysis in Sec. 5.3, we first check the new theoretical framework is able to reproduce results given in the literature by Rao et al. [22]. After confirming our simplified theoretical framework reproduces these results, we move to Sec. 5.3.1 where we once again calculate the entire spectrum of orbits for various scaled field values at the ionisation threshold ($E_c = 0$). Here we concentrate on the special cases of electrons launched in either the plane containing the electric field ($\phi = 0^\circ$) or the plane perpendicular to the electric field ($\phi = 90^\circ$).

As the scaled field is increased, the population of closed orbits diminishes substantially, especially in the high field regime at $f = 1$. Unlike the parallel fields case in Chap. 4 where the stability of the most stable four orbits at $f = 0$ increases with increasing scaled field, here their stability diminishes quite suddenly at high scaled field ($f = 1$) as these orbits generally no longer return close enough to the nucleus to be considered as closed orbits.

Next, as was investigated for the parallel fields case, we focus on the high field regime at $f = 1$, and increase the scaled energy in integer steps up to $E_c = 4$ to replicate the energies relevant in the case of silicon. As was discussed for the previous section, the orbits which are most stable at low fields now do not return close enough to the nucleus to be considered as closed, therefore, the most stable closed orbits in the high field regime tend to be new orbits not previously considered as important in other field configurations or low scaled fields. In focussing on the four most stable orbits at each integer value of the scaled energy, we identified many of these new orbits in both the $\phi = 0$ and $90^\circ$ planes. A large portion of these new orbits were also found to be composites of the most stable simpler orbits at low field values. Interestingly, for the $\phi = 90^\circ$ plane at high scaled field $f = 1$, and highest scaled energy $E_c = 4$, the three most stable orbits are once again represented by the most stable orbits at low scaled field and energy values.

As a consequence of the breaking of rotational symmetry with the application of an electric field perpendicular to the applied magnetic field, orbits no longer belong
to a family sharing the same polar launch angle, but varying azimuthal launch angle. In Sec. 5.3.3, we investigate the azimuthal angle dependence of the GT orbit, and its first seven harmonics. In rotationally symmetric external-field geometries, such as those investigated in Chaps. 2 and 4, this azimuthal dependence is absent. However, in the crossed fields geometry, this is not the case and the azimuthal dependence of orbits must be considered. We found that by introducing a weak electric field perpendicular to the applied magnetic field, the GT orbit, and its harmonics who lack rotational symmetry about the magnetic-field axis, show a two-fold azimuthal dependence. However, for harmonics which are essentially periodic, namely the third and sixth harmonics, a four-fold azimuthal dependence was observed. These rotationally symmetric harmonics were also more stable against increase in scaled field. We also found that the symmetries of the GT orbit, and its harmonics, were more sensitive to variations in scaled energy than scaled field.

In the course of the calculations, many bifurcation processes were observed where a continuum of essentially closed orbits were present over up to a third of the entire azimuthal angle range. As is the case with bifurcations in other field configurations, such as the orbit mixing observed for the case of parallel fields in Chap. 4, we expect these regions to present large resonances in experimental data. We also found here the possibility of a bifurcation reducing the azimuthal angle dependence of the third and sixth harmonics at $f = 0.25$ and small positive scaled energies. This is counter to all other bifurcation processes which were observed in our investigation.
Bibliography


Appendix A

Scaled field and energy variation for parallel electric and magnetic fields

In this appendix, we detail the complete effect on the whole system, and important individual orbits, of varying the scaled field and energy over all the values used throughout Chap 4. More precisely, we focus on the scaled fields of $f = 0, 0.01, 0.1, 1$ and scaled energies of $E_c = 0, 1, 2, 3, 4$. For each scaled field/energy combination, the whole spectrum of orbits, the most important individual orbits and their respective characteristics will be given.
Figure A.1: The return distance ($r_{ret}$) to the nucleus as a function of launch polar angle for various combinations of scaled field and scaled energy. Plots increase with scaled field from left to right with $f = 0, 0.01, 0.1, \text{ and } 1$ and increase with scaled energy from top to bottom with $E_c = 0, 1, 2, 3, \text{ and } 4$. Data points are shaded according to their orbital period in the range $0 - 5T_c$ as indicated by the bar at the bottom of the figure.
### APPENDIX A. PARALLEL-FIELDS ORBIT DEPENDENCIES

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**Table A.1**: The polar launch $\theta$, period $T/T_c$, return and maximum distances, and the bundle number $N_{\text{bun}}$, for different values of the parallel scaled field $f$ and scaled energy $\mathcal{E}_c$ for the orbit denoted as “Du1”.
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Figure A.2: The coordinate $z$ as a function of the cylindrical coordinate $\rho$ for the orbits evolving from the Garton-Tomkins orbit as the scaled field and energy are varied as in Table A.1. The scaled field increase from left to right with $f = 0, 0.01, 0.1, \text{ and } 1$, and the scaled energy increases from top to bottom with $\mathcal{E}_c = 0, 1, 2, 3, \text{ and } 4$. The point colour goes from red to blue as the electron describes the essentially closed path along the arrows shown. Colours representing the launch of the orbit in red are hidden when the curve overlaps itself.
Figure A.3: The $x$-$y$ view of the orbits in Fig. A.2.
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#### 152

**Du2 with positive launching z-component**

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| $\theta$ | $65.145^\circ$ | $64.946^\circ$ | $63.127^\circ$ | $40.616^\circ$ |
| $T/T_c$ | $1.65335$ | $1.65384$ | $1.65819$ | $1.69678$ |
| $r_{\text{ret}}/\lambda$ | $6.66 \times 10^{-9}$ | $7.38 \times 10^{-8}$ | $6.64 \times 10^{-8}$ | $3.79 \times 10^{-8}$ |
| $r_{\text{max}}/\lambda$ | $0.774199$ | $0.774895$ | $0.781439$ | $0.912468$ |
| $N_{\text{bun}}$ | $413$ | $416$ | $435$ | $927$ |

| $\theta$ | $71.439^\circ$ | $71.270^\circ$ | $69.732^\circ$ | $51.786^\circ$ |
| $T/T_c$ | $1.71812$ | $1.71851$ | $1.72191$ | $1.75212$ |
| $r_{\text{ret}}/\lambda$ | $5.80 \times 10^{-9}$ | $1.15 \times 10^{-7}$ | $1.09 \times 10^{-7}$ | $5.92 \times 10^{-8}$ |
| $r_{\text{max}}/\lambda$ | $0.859811$ | $0.860322$ | $0.865013$ | $0.945133$ |
| $N_{\text{bun}}$ | $286$ | $288$ | $300$ | $506$ |

| $\theta$ | $75.277^\circ$ | $75.128^\circ$ | $73.774^\circ$ | $58.362^\circ$ |
| $T/T_c$ | $1.76704$ | $1.76735$ | $1.77005$ | $1.79414$ |
| $r_{\text{ret}}/\lambda$ | $6.37 \times 10^{-8}$ | $2.47 \times 10^{-8}$ | $8.97 \times 10^{-9}$ | $2.65 \times 10^{-8}$ |
| $r_{\text{max}}/\lambda$ | $0.94842$ | $0.948816$ | $0.952496$ | $1.01163$ |
| $N_{\text{bun}}$ | $213$ | $214$ | $223$ | $347$ |

| $\theta$ | $77.798^\circ$ | $77.665^\circ$ | $76.443^\circ$ | $62.717^\circ$ |
| $T/T_c$ | $1.80397$ | $1.80419$ | $1.80639$ | $1.82605$ |
| $r_{\text{ret}}/\lambda$ | $2.10 \times 10^{-7}$ | $4.85 \times 10^{-8}$ | $5.19 \times 10^{-8}$ | $1.96 \times 10^{-8}$ |
| $r_{\text{max}}/\lambda$ | $1.0352$ | $1.03548$ | $1.03854$ | $1.08605$ |
| $N_{\text{bun}}$ | $167$ | $168$ | $174$ | $263$ |

**Table A.2:** The polar launch $\theta$, period $T/T_c$, return and maximum distances, and the bundle number $N_{\text{bun}}$, for different values of the parallel scaled field $f$ and scaled energy $\mathcal{E}_c$ for the orbit denoted as “Du2” launched with its $z$-component aligned with the applied fields.
As for Fig. A.2 but for the orbits given in Table A.2.

Figure A.4: As for Fig. A.2 but for the orbits given in Table A.2.
Figure A.5: The x - y view of the orbits in Fig. A.4.
APPENDIX A. PARALLEL-FIELDS ORBIT DEPENDENCIES

Du2 with negative launching $z$-component

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$r_{\text{ret}}/\lambda$

| 0                           | $1.11 \times 10^{-7}$ | $9.74 \times 10^{-9}$ | $6.90 \times 10^{-8}$ | $6.83 \times 10^{-8}$ |
| $r_{\text{max}}/\lambda$   | 0.707072              | 0.705907              | 0.696089              | 0.633792              |
| $N_{\text{bun}}$            | 680                   | 679                   | 637                   | 424                   |

$r_{\text{ret}}/\lambda$

| 1                           | $6.66 \times 10^{-9}$ | $1.04 \times 10^{-7}$ | $3.75 \times 10^{-8}$ | $1.27 \times 10^{-8}$ |
| $r_{\text{max}}/\lambda$   | 0.774199              | 0.773524              | 0.767602              | 0.725303              |
| $N_{\text{bun}}$            | 413                   | 411                   | 394                   | 282                   |

$r_{\text{ret}}/\lambda$

| 2                           | $5.80 \times 10^{-9}$ | $5.80 \times 10^{-8}$ | $1.38 \times 10^{-8}$ | $1.37 \times 10^{-7}$ |
| $r_{\text{max}}/\lambda$   | 0.859811              | 0.859324              | 0.855018              | 0.822794              |
| $N_{\text{bun}}$            | 286                   | 284                   | 273                   | 194                   |

$r_{\text{ret}}/\lambda$

| 3                           | $6.37 \times 10^{-8}$ | $9.18 \times 10^{-9}$ | $1.99 \times 10^{-8}$ | $3.12 \times 10^{-8}$ |
| $r_{\text{max}}/\lambda$   | 0.94842               | 0.948037              | 0.944639              | 0.91855               |
| $N_{\text{bun}}$            | 213                   | 212                   | 204                   | 141                   |

$r_{\text{ret}}/\lambda$

| 4                           | $2.21 \times 10^{-8}$ | $4.92 \times 10^{-8}$ | $1.46 \times 10^{-9}$ | $1.48 \times 10^{-7}$ |
| $r_{\text{max}}/\lambda$   | 1.03516               | 1.03483               | 1.03202               | 1.01009               |
| $N_{\text{bun}}$            | 167                   | 167                   | 159                   | 106                   |

Table A.3: The polar launch $\theta$, period $T/T_c$, return and maximum distances, and the bundle number $N_{\text{bun}}$, for different values of the parallel scaled field $f$ and scaled energy $\mathcal{E}_c$ for the orbit denoted as “Du2” launched with its $z$-component aligned against the applied fields.
Figure A.6: As for Fig. A.2 but for the orbits given in Table A.3.
Figure A.7: The $x$ - $y$ view of the orbits in Fig. A.6.
### APPENDIX A. PARALLEL-FIELDS ORBIT DEPENDENCIES

#### Du3 with positive launching z-component

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<td>315</td>
<td>383</td>
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</tr>
<tr>
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<td>54.039°</td>
<td>-</td>
</tr>
<tr>
<td>$T/T_c$</td>
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<td>2.65417</td>
<td>2.66294</td>
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</tr>
<tr>
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<td>$1.20 \times 10^{-8}$</td>
<td>$3.84 \times 10^{-8}$</td>
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</tr>
<tr>
<td>$r_{\text{max}}/\lambda$</td>
<td>1.14295</td>
<td>1.14635</td>
<td>1.17822</td>
<td>-</td>
</tr>
<tr>
<td>$N_{\text{bun}}$</td>
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<td>194</td>
<td>-</td>
</tr>
<tr>
<td>$\theta$</td>
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</tr>
<tr>
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<td>2.71114</td>
<td>2.7185</td>
<td>2.77808</td>
</tr>
<tr>
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<td>$1.04 \times 10^{-7}$</td>
<td>$4.38 \times 10^{-9}$</td>
<td>$1.30 \times 10^{-5}$</td>
</tr>
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<td>1.22027</td>
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<td>546</td>
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<td>69.404°</td>
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<td>43.622°</td>
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<td>2.76161</td>
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<td>$8.91 \times 10^{-8}$</td>
<td>$1.05 \times 10^{-7}$</td>
</tr>
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<td>1.2677</td>
<td>1.69403</td>
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<tr>
<td>$N_{\text{bun}}$</td>
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<td>94</td>
<td>103</td>
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<td>72.733°</td>
<td>71.060°</td>
<td>50.195°</td>
</tr>
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<td>$T/T_c$</td>
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<td>2.78969</td>
<td>2.79511</td>
<td>2.83834</td>
</tr>
<tr>
<td>$r_{\text{ret}}/\lambda$</td>
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<td>$1.97 \times 10^{-7}$</td>
<td>$1.40 \times 10^{-7}$</td>
<td>$6.48 \times 10^{-9}$</td>
</tr>
<tr>
<td>$r_{\text{max}}/\lambda$</td>
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<td>1.29063</td>
<td>1.31863</td>
<td>1.73337</td>
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<td>$N_{\text{bun}}$</td>
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**Table A.4:** The polar launch $\theta$, period $T/T_c$, return and maximum distances, and the bundle number $N_{\text{bun}}$, for different values of the parallel scaled field $f$ and scaled energy $\mathcal{E}_c$ for the orbit denoted as “Du2” launched with its $z$-component aligned with the applied fields.
APPENDIX A. PARALLEL-FIELDS ORBIT DEPENDENCIES

As for Fig. A.2 but for the orbits given in Table A.4.

Figure A.8: As for Fig. A.2 but for the orbits given in Table A.4.
Figure A.9: The x - y view of the orbits in Fig. A.8.
### Table A.5: The polar launch $\theta$, period $T/T_c$, return and maximum distances, and the bundle number $N_{\text{bun}}$, for different values of the parallel scaled field $f$ and scaled energy $E_c$ for the orbit denoted as “Du3” launched with its $z$-component aligned against the applied fields.

<table>
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<td>$\theta$</td>
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<td>133.583°</td>
<td>109.787°</td>
</tr>
<tr>
<td>$T/T_c$</td>
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<td>2.56998</td>
<td>2.44959</td>
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<tr>
<td>$r_{\text{ret}}/\lambda$</td>
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<td>$6.55 \times 10^{-8}$</td>
<td>$4.93 \times 10^{-8}$</td>
</tr>
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<td>$r_{\text{max}}/\lambda$</td>
<td>1.10748</td>
<td>1.10396</td>
<td>1.0735</td>
<td>0.85798</td>
</tr>
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<td>$N_{\text{bun}}$</td>
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</tr>
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<td>$\theta$</td>
<td>123.133°</td>
<td>122.859°</td>
<td>120.465°</td>
<td>101.177°</td>
</tr>
<tr>
<td>$T/T_c$</td>
<td>2.65321</td>
<td>2.65218</td>
<td>2.64319</td>
<td>2.54127</td>
</tr>
<tr>
<td>$r_{\text{ret}}/\lambda$</td>
<td>$6.90 \times 10^{-9}$</td>
<td>$8.45 \times 10^{-8}$</td>
<td>$6.54 \times 10^{-8}$</td>
<td>$4.46 \times 10^{-8}$</td>
</tr>
<tr>
<td>$r_{\text{max}}/\lambda$</td>
<td>1.14295</td>
<td>1.13955</td>
<td>1.11026</td>
<td>0.906536</td>
</tr>
<tr>
<td>$N_{\text{bun}}$</td>
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<td>152</td>
<td>65</td>
</tr>
<tr>
<td>$\theta$</td>
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<td>115.071°</td>
<td>113.059°</td>
<td>96.379°</td>
</tr>
<tr>
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<td>2.71028</td>
<td>2.7095</td>
<td>2.70183</td>
<td>2.61708</td>
</tr>
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<td>$8.13 \times 10^{-8}$</td>
<td>$4.20 \times 10^{-8}$</td>
<td>$2.69 \times 10^{-10}$</td>
<td>$9.41 \times 10^{-7}$</td>
</tr>
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<td>$r_{\text{max}}/\lambda$</td>
<td>1.18635</td>
<td>1.18314</td>
<td>1.15506</td>
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</tr>
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<td>$N_{\text{bun}}$</td>
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<td>109</td>
<td>47</td>
</tr>
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<td>$\theta$</td>
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<td>110.194°</td>
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<td>93.577°</td>
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<tr>
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<td>2.75469</td>
<td>2.75307</td>
<td>2.74748</td>
<td>2.67684</td>
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<tr>
<td>$r_{\text{ret}}/\lambda$</td>
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<td>$6.03 \times 10^{-8}$</td>
<td>$4.41 \times 10^{-8}$</td>
<td>$9.14 \times 10^{-7}$</td>
</tr>
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<td>1.2322</td>
<td>1.2055</td>
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<td>92</td>
<td>85</td>
<td>36</td>
</tr>
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<td>$\theta$</td>
<td>107.085°</td>
<td>106.904°</td>
<td>105.303°</td>
<td>91.853°</td>
</tr>
<tr>
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<td>2.7885</td>
<td>2.78296</td>
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<td>$r_{\text{ret}}/\lambda$</td>
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<td>$9.65 \times 10^{-9}$</td>
<td>$1.36 \times 10^{-7}$</td>
<td>$9.47 \times 10^{-7}$</td>
</tr>
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<td>$r_{\text{max}}/\lambda$</td>
<td>1.28767</td>
<td>1.28475</td>
<td>1.25949</td>
<td>1.09936</td>
</tr>
<tr>
<td>$N_{\text{bun}}$</td>
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<td>75</td>
<td>69</td>
<td>28</td>
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APPENDIX A. PARALLEL-FIELDS ORBIT DEPENDENCIES

Figure A.10: As for Fig. A.2 but for the orbits given in Table A.5.
Figure A.11: The x-y view of the orbits in Fig. A.10.
### APPENDIX A. PARALLEL-FIELDS ORBIT DEPENDENCIES

**Table A.6:** The polar launch $\theta$, period $T/T_c$, return and maximum distances, and the bundle number $N_{bun}$, for different values of the parallel scaled field $f$ and scaled energy $E_c$ for the orbit denoted as “Du4” launched with its $z$-component aligned with the applied fields.

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<th>$f = 1$</th>
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</thead>
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<td>$\theta$</td>
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<tr>
<td>$T/T_c$</td>
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<td>2.14512</td>
<td>2.1444</td>
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<td>7.82 $\times$ 10$^{-8}$</td>
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<td>0.643456</td>
<td>0.648843</td>
<td>0.724737</td>
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<td>237</td>
<td>238</td>
<td>409</td>
</tr>
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<td>$\theta$</td>
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<td>70.745°</td>
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<td>48.103°</td>
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<tr>
<td>$T/T_c$</td>
<td>2.39928</td>
<td>2.39932</td>
<td>2.399</td>
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</tr>
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<td>$r_{ret}/\lambda$</td>
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<td>7.94 $\times$ 10$^{-8}$</td>
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</tr>
<tr>
<td>$r_{max}/\lambda$</td>
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<td>2.54326</td>
<td>2.5431</td>
<td>2.52946</td>
</tr>
<tr>
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<td>7.77 $\times$ 10$^{-8}$</td>
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<td>$r_{max}/\lambda$</td>
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<td>0.839591</td>
<td>0.843008</td>
<td>0.899922</td>
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<tr>
<td>$N_{bun}$</td>
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<td>63</td>
<td>66</td>
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<tr>
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<td>2.70113</td>
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</table>
Figure A.12: As for Fig. A.2 but for the orbits given in Table A.6.
Figure A.13: The $x$ - $y$ view of the orbits in Fig. A.12.
### Table A.7: The polar launch $\theta$, period $T/T_c$, return and maximum distances, and the bundle number $N_{\text{bun}}$, for different values of the parallel scaled field $f$ and scaled energy $E_c$ for the orbit denoted as “Du4” launched with its $z$-component aligned against the applied fields.

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<td>2.14514</td>
<td>2.14439</td>
<td>2.04663</td>
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<td>$8.32 \times 10^{-8}$</td>
<td>$7.91 \times 10^{-8}$</td>
<td>$6.97 \times 10^{-8}$</td>
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<td>239</td>
<td>408</td>
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<td>$\theta$</td>
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<td>107.132°</td>
<td>91.368°</td>
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<td>2.39929</td>
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<td>$\theta$</td>
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<td>2.54322</td>
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<td>$2.23 \times 10^{-9}$</td>
<td>$2.77 \times 10^{-8}$</td>
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<td>$1.24 \times 10^{-7}$</td>
<td>$4.77 \times 10^{-7}$</td>
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<tr>
<td>$\theta$</td>
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<td>2.70113</td>
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</table>
Figure A.14: As for Fig. A.2 but for the orbits given in Table A.7.
**APPENDIX A. PARALLEL-FIELDS ORBIT DEPENDENCIES**

Figure A.15: The $x$ - $y$ view of the orbits in Fig. A.14.
Appendix B

Scaled field and energy variation for crossed electric and magnetic fields

In this appendix, we detail the complete effect on the whole system, and important individual orbits, of varying the scaled field and energy over all the values used throughout Chap 5. More precisely, we focus on the scaled fields of $f = 0, 0.01, 0.1,$ and 1 and scaled energies of $E_c = 0, 1, 2, 3,$ and 4. For each scaled field/energy combination, the whole spectrum of orbits, the most important individual orbits and their respective characteristics will be given.

B.1 $\phi = 0^\circ$ azimuthal plane
Figure B.1: The return distance ($r_{\text{ret}}$) to the nucleus as a function of launch polar angle for various combinations of scaled field and scaled energy for orbits launched in the $\phi = 0^\circ$ plane. Plots increase with scaled field from left to right with $f = 0, 0.01, 0.1, \text{ and } 1$ and increase with scaled energy from top to bottom with $E_c = 0, 1, 2, 3, \text{ and } 4$. Data points are shaded according to their orbital period in the range $0 - 5T_c$ as indicated by the bar at the bottom of the figure. Panel (t) is zoomed in an extra two orders of magnitude to reveal the only closed orbit of the system at $f = 1$ and $E_c = 4$. 

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### Table B.1: The polar launch $\theta$, period $T/T_c$, return and maximum distances, and the bundle number $N_{bun}$, for different values of the parallel scaled field $f$ and scaled energy $E_c$ for the orbit denoted as “Du1” launched in the $\phi = 0^\circ$ azimuthal plane.

<table>
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<th>$f = 1$</th>
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<td>$90^\circ$</td>
<td>$90^\circ$</td>
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</tr>
<tr>
<td>$T/T_c$</td>
<td>0.666667</td>
<td>0.666003</td>
<td>0.660125</td>
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<tr>
<td>$r_{\text{ret}}/\lambda$</td>
<td>$1.23 \times 10^{-8}$</td>
<td>$2.30 \times 10^{-6}$</td>
<td>$2.20 \times 10^{-4}$</td>
<td>-</td>
</tr>
<tr>
<td>$r_{\text{max}}/\lambda$</td>
<td>0.587368</td>
<td>0.586742</td>
<td>0.581168</td>
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</tr>
<tr>
<td>$N_{bun}$</td>
<td>2663</td>
<td>2668</td>
<td>2414</td>
<td>-</td>
</tr>
<tr>
<td>$\theta$</td>
<td>$90^\circ$</td>
<td>$90^\circ$</td>
<td>$90^\circ$</td>
<td>-</td>
</tr>
<tr>
<td>$T/T_c$</td>
<td>0.745493</td>
<td>0.744942</td>
<td>0.740115</td>
<td>-</td>
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<tr>
<td>$r_{\text{ret}}/\lambda$</td>
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<td>$4.26 \times 10^{-6}$</td>
<td>$4.04 \times 10^{-4}$</td>
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<tr>
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<tr>
<td>$T/T_c$</td>
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<td>$6.20 \times 10^{-4}$</td>
<td>-</td>
</tr>
<tr>
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<td>0.808916</td>
<td>0.802179</td>
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<td>$N_{bun}$</td>
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<td>671</td>
<td>-</td>
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<td>$\theta$</td>
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<td>-</td>
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<td>613</td>
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APPENDIX B. CROSSED-FIELDS ORBIT DEPENDENCIES

Figure B.2: The coordinate $z$ as a function of the cylindrical coordinate $\rho$ for the orbits evolving from the Garton-Tomkins orbit as the scaled field and energy are varied as in Table B.1. The scaled field increase from left to right with $f = 0, 0.01, 0.1, 1$, and the scaled energy increases from top to bottom with $\Sigma_c = 0, 1, 2, 3, 4$. The point colour goes from red to blue as the electron describes the essentially closed path along the arrows shown. Colours representing the launch of the orbit in red are hidden when the curve overlaps itself.
Figure B.3: The $x$-$y$ view of the orbits in Fig. B.2.
Table B.2: The polar launch $\theta$, period $T/T_c$, return and maximum distances, and the bundle number $N_{\text{bun}}$, for different values of the parallel scaled field $f$ and scaled energy $E_c$ for the orbit denoted as “Du2” launched in the $\phi = 0^\circ$ azimuthal plane.
Figure B.4: As for Fig. B.2 but for the orbits given in Table B.2.
FIGURE B.5: The $x$-$y$ view of the orbits in Fig. B.4.
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<td>40.993°</td>
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<tr>
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<td>2.57934</td>
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<td>$N_{\text{bun}}$</td>
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<td>$\theta$</td>
<td>56.867°</td>
<td>56.832°</td>
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<td></td>
</tr>
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<td>$T/T_c$</td>
<td>2.65321</td>
<td>2.65127</td>
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</tr>
<tr>
<td>$r_{\text{ret}}/\lambda$</td>
<td>$6.90 \times 10^{-8}$</td>
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<td>73</td>
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Table B.3: The polar launch $\theta$, period $T/T_c$, return and maximum distances, and the bundle number $N_{\text{bun}}$, for different values of the parallel scaled field $f$ and scaled energy $\mathcal{E}_c$ for the orbit denoted as “Du3” launched in the $\phi = 0^\circ$ azimuthal plane.
Figure B.6: As for Fig. B.2 but for the orbits given in Table B.3.
Figure B.7: The $x$ - $y$ view of the orbits in Fig. B.6.
<table>
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<th>$f = 1$</th>
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<td>63.647°</td>
<td>63.635°</td>
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</tr>
<tr>
<td></td>
<td>$T/T_c$</td>
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<td>2.10329</td>
<td>-</td>
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<td>$2.62 \times 10^{-5}$</td>
<td>-</td>
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<tr>
<td></td>
<td>$r_{max}/\lambda$</td>
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<td>0.636107</td>
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</tr>
<tr>
<td></td>
<td>$N_{bun}$</td>
<td>236</td>
<td>239</td>
<td>249</td>
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<tr>
<td></td>
<td>$\theta$</td>
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<td>70.928°</td>
<td>70.825°</td>
<td>70.583°</td>
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<tr>
<td></td>
<td>$T/T_c$</td>
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<td>105</td>
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<td>0.838503</td>
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<td>78.389°</td>
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<tr>
<td></td>
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<td></td>
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<td>2.70113</td>
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<td>$N_{bun}$</td>
<td>33</td>
<td>31</td>
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**Table B.4:** The polar launch $\theta$, period $T/T_c$, return and maximum distances, and the bundle number $N_{bun}$, for different values of the parallel scaled field $f$ and scaled energy $E_c$ for the orbit denoted as “Du4” launched in the $\phi = 0^\circ$ azimuthal plane.
Figure B.8: As for Fig. B.2 but for the orbits given in Table B.4.
Figure B.9: The $x$-$y$ view of the orbits in Fig. B.8.
B.2 $\phi = 90^\circ$ azimuthal plane
Figure B.10: The return distance \( r_{\text{ret}} \) to the nucleus as a function of launch polar angle for various combinations of scaled field and scaled energy for orbits launched in the \( \phi = 90^\circ \) plane. Plots increase with scaled field from left to right with \( f = 0, 0.01, 0.1, \) and 1 and increase with scaled energy from top to bottom with \( E_c = 0, 1, 2, 3, \) and 4. Data points are shaded according to their orbital period in the range 0–5\( T_c \) as indicated by the bar at the bottom of the figure. Panel (l) is missing due to their being no closed orbits for the system at \( f = 1 \) and \( E_c = 2 \).
### Table B.5: The polar launch $\theta$, period $T/T_c$, return and maximum distances, and the bundle number $N_{\text{bun}}$, for different values of the parallel scaled field $f$ and scaled energy $E_c$ for the orbit denoted as “Du1” launched in the $\phi = 90^\circ$ azimuthal plane.
Figure B.11: The coordinate $z$ as a function of the cylindrical coordinate $\rho$ for the orbits evolving from the Garton-Tomkins orbit as the scaled field and energy are varied as in Table B.5. The scaled field increase from left to right with $f = 0, 0.01, 0.1, 1$, and the scaled energy increases from top to bottom with $\mathcal{E}_c = 0, 1, 2, 3, 4$. The point colour goes from red to blue as the electron describes the essentially closed path along the arrows shown. Colours representing the launch of the orbit in red are hidden when the curve overlaps itself.
Figure B.12: The $x$-$y$ view of the orbits in Fig. B.11.
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<th>$\theta$</th>
<th>$T/T_c$</th>
<th>$r_{\text{ret}}/\lambda$</th>
<th>$r_{\text{max}}/\lambda$</th>
<th>$N_{\text{bun}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$0$</td>
<td>$53.832^\circ$</td>
<td>$53.823^\circ$</td>
<td>$52.723^\circ$</td>
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<td>$1$</td>
<td>$65.145^\circ$</td>
<td>$65.137^\circ$</td>
<td>$65.144^\circ$</td>
<td>$\phi = 0$</td>
<td>-</td>
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<td>$2$</td>
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<td>$71.439^\circ$</td>
<td>$71.435^\circ$</td>
<td>$\phi = 0$</td>
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<td>$3$</td>
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<td>$75.277^\circ$</td>
<td>$75.283^\circ$</td>
<td>$\phi = 0$</td>
<td>-</td>
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<tr>
<td>$4$</td>
<td>$77.798^\circ$</td>
<td>$77.800^\circ$</td>
<td>$77.809^\circ$</td>
<td>$\phi = 0$</td>
<td>-</td>
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Table B.6: The polar launch $\theta$, period $T/T_c$, return and maximum distances, and the bundle number $N_{\text{bun}}$, for different values of the parallel scaled field $f$ and scaled energy $E_c$ for the orbit denoted as “Du2” launched in the $\phi = 90^\circ$ azimuthal plane.
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Figure B.13: As for Fig. B.11 but for the orbits given in Table B.6.
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Figure B.14: The $x$-$y$ view of the orbits in Fig. B.13.
### Table B.7: The polar launch $\theta$, period $T/T_c$, return and maximum distances, and the bundle number $N_{\text{bun}}$, for different values of the parallel scaled field $f$ and scaled energy $\mathcal{E}_c$ for the orbit denoted as “Du3” launched in the $\phi = 90^\circ$ azimuthal plane.

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<th>Parameters</th>
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<tr>
<td></td>
<td>$\theta$</td>
<td>42.810°</td>
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<tr>
<td></td>
<td>$T/T_c$</td>
<td>2.58188</td>
<td>2.58413</td>
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<td>0</td>
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<tr>
<td></td>
<td>$r_{\text{max}}/\lambda$</td>
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<td>1.10811</td>
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APPENDIX B. CROSSED-FIELDS ORBIT DEPENDENCIES

Figure B.15: As for Fig. B.11 but for the orbits given in Table B.7.

\[\begin{align*}
\text{Du3, } f = 0, \epsilon_e = 0 & & \text{Du3, } f = 0.01, \epsilon_e = 0 \\
\theta = 42.810^\circ & & \theta = 42.799^\circ \\
T/T_C = 2.58388 & & T/T_C = 2.5843 \\
\rho/\lambda & & \rho/\lambda \\
-1.2 - 0.6 & 0 & 0.6 & 1.2 & -1.2 - 0.6 & 0 & 0.6 & 1.2 \\
\text{Du3, } f = 0, \epsilon_e = 1 & & \text{Du3, } f = 0.01, \epsilon_e = 1 \\
\theta = 56.867^\circ & & \theta = 56.864^\circ \\
T/T_C = 2.65321 & & T/T_C = 2.65444 \\
\rho/\lambda & & \rho/\lambda \\
-1.2 - 0.6 & 0 & 0.6 & 1.2 & -1.2 - 0.6 & 0 & 0.6 & 1.2 \\
\text{Du3, } f = 0, \epsilon_e = 2 & & \text{Du3, } f = 0.01, \epsilon_e = 2 \\
\theta = 64.701^\circ & & \theta = 64.700^\circ \\
T/T_C = 2.71028 & & T/T_C = 2.7115 \\
\rho/\lambda & & \rho/\lambda \\
-1.2 - 0.6 & 0 & 0.6 & 1.2 & -1.2 - 0.6 & 0 & 0.6 & 1.2 \\
\text{Du3, } f = 0, \epsilon_e = 3 & & \text{Du3, } f = 0.01, \epsilon_e = 3 \\
\theta = 69.605^\circ & & \theta = 69.606^\circ \\
T/T_C = 2.75469 & & T/T_C = 2.75508 \\
\rho/\lambda & & \rho/\lambda \\
-1.2 - 0.6 & 0 & 0.6 & 1.2 & -1.2 - 0.6 & 0 & 0.6 & 1.2 \\
\text{Du3, } f = 0, \epsilon_e = 4 & & \text{Du3, } f = 0.01, \epsilon_e = 4 \\
\theta = 72.915^\circ & & \theta = 72.916^\circ \\
T/T_C = 2.78909 & & T/T_C = 2.79034 \\
\rho/\lambda & & \rho/\lambda \\
-1.2 - 0.6 & 0 & 0.6 & 1.2 & -1.2 - 0.6 & 0 & 0.6 & 1.2 \\
\end{align*}\]
Figure B.16: The $x$-$y$ view of the orbits in Fig. B.15.
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**Table B.8:** The polar launch $\theta$, period $T/T_c$, return and maximum distances, and the bundle number $N_{bun}$, for different values of the parallel scaled field $f$ and scaled energy $\mathcal{E}_c$ for the orbit denoted as “Du4” launched in the $\phi = 90^\circ$ azimuthal plane.
Figure B.17: As for Fig.B.11 but for the orbits given in Table B.8.
Figure B.18: The $x$-$y$ view of the orbits in Fig. B.17.