Hamiltonian Study of the Toroidal Helical Magnetic Field in the Vacuum with Symplectic Integrators

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Abstract

It is well known that the magnetic field lines system can be treated as a Hamiltonian system, however a full exploitation of this fact has been hindered by the difficulty of finding the proper canonical variables or by their inconvenience for the solution of practical problems. There would be many advantages in having a Hamiltonian formulation of the problem of the magnetic field lines flow, because for Hamiltonian systems many theoretical results, like for example conservation theorems, are known. Moreover, in recent years the so called symplectic numerical integration schemes have been developed, and these schemes are particularly designed for Hamiltonian dynamical systems. These methods are very important for the magnetic field lines problem, because to obtain a detailed description of the field lines system it is necessary to follow their winding around the torus many times, typically for $10^5 \sim 10^6$ revolutions, and this results, when traditional integration methods like the Runge-Kutta are used, in the accumulation of secular errors that make the results unreliable. On the other hand, symplectic methods are free from secular errors.

In this thesis we investigate possible Hamiltonian formulations for the toroidal helical

magnetic field in the vacuum and study the obtained models by means of a new linear symplectic integration scheme developed by us.

We first derive a Hamiltonian for the cylindrical limit approximation of the field. The Hamiltonian is derived until the second perturbative order and it is obtained by using a perturbation theory based on the Lie transform. This perturbation theory is a theory in which all the relations are expressed in operational form, resulting in superior efficiency and compactness when compared to the classical perturbation theory. The Lie transform based perturbation theory forms the core of our theoretical study of all the Hamiltonian models treated in this thesis.

We then study the general toroidal case and derive for it two different Hamiltonian models, the first one correct until the third perturbative order, the second one correct until the second. The second model is an integrable model, while the first one is not. This apparent discrepancy is connected with the use of the perturbation expansion and can be explained by noticing that the canonical variables used for the two models are different. Moreover, the perturbation theory yields expressions that are only asymptotic, so some care must be exercised when using it. The second, integrable model, of course is not able to reproduce the chaotic region of the real field, but in the first model we are able to show that the characteristic formation of magnetic surfaces, islands and chaotic regions is reproduced. We therefore proceed to the development of a new linear symplectic integration method. This has been motivated by the observation that most of the symplectic methods existing

in the literature are intended for quite special Hamiltonian systems and are therefore not useful in our case. The ideas underlining its construction are explained, and stability and accuracy analyses are also presented. Finally we present the numerical results, showing that the third order Hamiltoninan is able to fully reproduce the regular and chaotic regions of the toroidal helical field. The present study concludes that the Hamiltonian approach is feasible and that a suitable Hamiltonian integrated by a symplectic method can be a cheap way to study with good accuracy the transition region between order and chaos.

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Chapter 1

Introduction

1.1 The Reasons of this Work

The toroidal helical magnetic field possesses magnetic surfaces in the proximity of the magnetic axis, while in regions far from the magnetic axis such surfaces do not exist. The domain in which magnetic surfaces do not exist is called magnetic chaos domain, and between the magnetic axis and the magnetic chaos domain lies the outermost magnetic surface, whose position is an important information from the point of view of magnetic confinement.

Since the divergence of the magnetic field is zero, the magnetic field lines system can be treated as a Hamiltonian system. For Hamiltonian systems the phase space structure is subdivided into chaotic and regular regions, and this subdivision has a correspondence

with the magnetic chaos domain and the magnetic surfaces domain discussed above.

The existing research in this field is based on numerical calculations about the structure of the magnetic field, but in these methods numerical errors are inherently present and this poses limitations on the accuracy by which the properties of the outermost magnetic surface are investigated. To enhance the accuracy it is necessary to track many times the magnetic field lines around the torus, typically for $10^5 \sim 10^6$ revolutions, but there are indications that this procedure causes a shrink of the surface towards the magnetic axis and that the accumulation of secular errors makes the interpretation of the results problematic. A possible explanation of this fact is that the divergence-free nature of the magnetic field is not fully respected in these numerical methods. In other words, many numerical calculations do not respect the intrinsic Hamiltonian nature of the magnetic field lines system, in the sense that the numerical schemes utilized are not symplectic, while the flow of the magnetic field lines system is symplectic. With this background in mind, we think that in order to further advance this kind of research it is necessary to approach the problem from the point of view of Hamiltonian theory, in which the divergence-free property is rigorously respected. Besides, it is important to notice that for Hamiltonian systems it is possible to use symplectic integration techniques to solve the equation of motion, techniques which are free from secular, or dissipative errors. Symplectic integration schemes have been developed in the past few years and seem to be the best way to numerically investigate the properties of Hamiltonian systems.

The research approaching the toroidal helical magnetic field problem from the Hamiltonian point of view ends with works done more than ten years ago (refs. [1], [2] and [3]), partly because of the strong push towards research on tokamaks. However, we have two good reasons to revive the Hamiltonian approach to the toroidal helical magnetic field problem:

1). The Japanese Ministry of Education is pushing the research concerning the helical systems approach to magnetic confinement and the LHD (Large Helical Device) is in phase of construction.

2). The last ten years have seen an impetuous development of chaos physics, and time is ripe for research about the chaotic properties of the toroidal helical magnetic field lines system.

Recently T. Hatori and T. Watanabe (ref. [4]) have obtained an explicit form for the Boozer's magnetic coordinates in the first order toroidal correction to the cylindrical helical magnetic configuration. In this work a more systematic procedure (Lie perturbation expansion technique) is used to proceed to higher orders and a new linear symplectic method is constructed and used to integrate numerically the equations of motion.

1.2 Overview

The remaining part of this thesis is subdivided into five chapters and an appendix.

In chapter 2 we first review those concepts from Hamiltonian mechanics which will be relevant to our work and describe the Hamiltonian nature of the magnetic field lines system. Then the concept of Lie transform is introduced and its utilization for a perturbation theory that is more efficient than the classical one is described.

In chapter 3 we present the calculations that allow us to construct a Hamiltonian for the magnetic field lines system. The Hamiltonian is obtained for the cylindrical approximation of the field and for the toroidal case.

In chapter 4 we will discuss in detail symplectic integration schemes and the development of a new linear symplectic integration scheme which will be used to solve the Hamilton's equations derived in chapter 3.

In chapter 5 some numerical results and their discussion is presented. Of particular interest is that our Hamiltonian, yet of simple form, is able to reproduce fully the regular and the chaotic region of the field.

In chapter 6 the concluding remarks are given.

In the appendix the coefficients that characterize our method are explicitly calculated.

1.2.1 Notation

We have tried to avoid a rigorous, but heavy notation, in the the hope that the context will help the reader to decipher the notation. We do not use boldface character for vectors, so a symbol like p could indicate a single variable or the vector $(p_1, \ldots, p_n)$. The Einstein summation convention is used extensively. When the indexes are Latin the sum is from 1, when the indexes are Greek the sum is from 0. For the partial derivative both the symbols $\frac{\partial}{\partial x}$ and ∂_x are used.

Chapter 2

The Lie Transform

2.1 Introduction

In this chapter we will first review those aspects of Hamiltonian mechanics which will be relevant to our work. In particular the notion of canonical transformation and the symplectic nature of the flow of Hamiltonian systems will be described. Then the equation for the magnetic field lines will be put into a form which is equivalent to Hamilton's equation. In the final section the concept of Lie transform will be introduced. The Lie transform can be used as a basis for a perturbation theory which is more efficient and elegant than the classical one.

2.2 Hamiltonian Mechanics

In classical mechanics a system of N particles is described by the Newton equations

$$m_i \ddot{r}_i = F_i \tag{2.1}$$

where $i = 1, \ldots, N$ and F_i is the total force acting on the ith point of mass m_i. If constraints that limit the motion of the system are present (for example the motion may be constrained to occur on some surface or curve), then the coordinates $r_1, \ldots, r_N$ are not independent of each other. However, if the constraints are holonomic, that is if they are expressible by equations of the type

$$f_j(r_1, \ldots, r_N, t) = 0, \qquad j = 1, \ldots, K, \tag{2.2}$$

then it is possible to change the coordinates from $r_1, \ldots, r_N$ to a new set of independent coordinates $q_1, \ldots, q_n$, with $n = 3N - K$, which are called generalized coordinates. For conservative systems, that is for systems such that the forces are derivable from the gradient of a potential function $V(r_1, \ldots, r_N)$, then a Lagrangian $L(q_1, \ldots, q_n) = T - V$, where T is the total kinetic energy of the system, can be constructed, [1] and the equations of motion for the generalized coordinates are given by

$$\frac{d}{dt}\frac{\partial}{\partial \dot{q}_j} L - \frac{\partial}{\partial q_j} L = 0. \tag{2.3}$$

[1] We observe that a Lagrangian can be constructed also for the electromagnetic forces on moving charges, though in that case the forces are derivable from a velocity-dependent potential.

Once a Lagrangian has been constructed for a given system, we can construct the Hamiltonian function H, defined as

$$H(q,p,t) = \sum \dot{q}_i p_i - L(q,\dot{q},t), \tag{2.4}$$

where $p = p_1,\ldots,p_n$ are called generalized momenta and are defined by $p_i = \frac{\partial}{\partial \dot{q}_i} L$. By this procedure the n coordinates $q_1,\ldots,q_n$ are substituted by the $2n$ coordinates $q_1,\ldots,q_n,p_1,\ldots,p_n$ and the n, second order Lagrange equations by the $2n$, first order Hamilton equations

$$\dot{q}_i = \frac{\partial}{\partial p_i} H, \qquad \dot{p}_i = -\frac{\partial}{\partial q_i} H. \tag{2.5}$$

The Hamilton equations can be derived also from the variational principle

$$\delta \int dt(\sum p_i \dot{q}_i - H(q,p,t)) = 0. \tag{2.6}$$

This variational principle will allow us to compare the equations for the magnetic field line flow with the Hamilton equations and to identify the magnetic field line system as a Hamiltonian system.

Solving analytically the Hamilton equations is in general not possible except in very special, though very important, cases. Often it is useful, even if we want to proceed to a numerical integration of eqs. (2.5), to make a transformation of variables in order to simplify the equations or in order to reveal some symmetry of the physical system.

However, when we transform the coordinates from $q = (q_1, q_2, ..., q_n)$, $p = (p_1, p_2, ..., p_n)$ to $Q = (Q_1, Q_2, ..., Q_N)$, $P = (P_1, P_2, ..., P_N)$, it is desirable that the equations of motion

in the new variables Q, P be in the same form as (2.5), that is there must exist a function $K(Q,P,t)$ such that $\dot{Q}_i = \frac{\partial}{\partial P_i} K$, $\dot{P}_i = -\frac{\partial}{\partial Q_i} K$, which is in general not true for arbitrary coordinate transformation. A transformation which preserves the form of Hamilton's equations is called a canonical transformation. We now state the conditions under which the transformation

$$Q_i = Q_i(q_1,...,p_n), \quad P_i = P_i(q_1,...,p_n), \tag{2.7}$$

is canonical. If M is the Jacobian of the transformation (2.7)

$$M = \begin{pmatrix} \frac{\partial}{\partial q} Q & \frac{\partial}{\partial q} P \\ \frac{\partial}{\partial p} Q & \frac{\partial}{\partial p} P \end{pmatrix},$$

and J the skew-symmetrical matrix

$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}, \tag{2.8}$$

then a necessary and sufficient condition for the transformation (2.7) to be canonical is that the condition $M^t J M = J$ is satisfied (ref. [5], pag. 391-397). This condition is called symplectic condition.

While when changing coordinates it is often convenient to change coordinates by means of a canonical transformation, this is not strictly necessary, for some systems are better understood using noncanonical variables. However canonical transformations manifest their importance when we consider the time evolution of the system. In fact, let us suppose that $q = q(q_0, p_0, t)$ and $p = p(q_0, p_0, t)$ are a solution of Hamilton's equations. Then it can be

shown that the coordinate transformation $(q_0, p_0) \to (q, p)$ is a canonical transformation, that is the symplectic condition $M^t J M = J$ holds, where

$$M = \begin{pmatrix} \frac{\partial}{\partial q_0} q & \frac{\partial}{\partial q_0} p \\ \frac{\partial}{\partial p_0} q & \frac{\partial}{\partial p_0} p \end{pmatrix}.$$

The time evolution of a Hamiltonian system satisfies therefore the symplectic condition, and this fact has important practical consequences, as we will see when we discuss symplectic integration methods.

An important property of Hamiltonian systems is the conservation of phase space volume, a fact known as Liouville theorem. Liouville theorem is easily proved: if we define a velocity vector $v = (q, p)$, then the divergence of this vector is

$$\begin{aligned} \nabla \cdot v &= \frac{\partial}{\partial q_i}\dot{q}_i + \frac{\partial}{\partial p_i}\dot{p}_i \\ &= \frac{\partial}{\partial q_i}\frac{\partial}{\partial p_i}H - \frac{\partial}{\partial p_i}\frac{\partial}{\partial q_i}H = 0, \end{aligned} \tag{2.9}$$

that is, if we consider the motion of the points of the phase space as composing a fluid, this fluid is incompressible. Actually the conservation of phase space volume is a particular case of a more general theorem, which says that the flow of a Hamiltonian system preserves the differential form $\omega = dp^1 \wedge dq^1 + \cdots + dp^n \wedge dq^n$ and the exterior powers $\omega^2, \ldots, \omega^n$. [2] This theorem is equivalent to the fact that the time evolution of a Hamiltonian system satisfies the symplectic condition. The Liouville theorem corresponds to the conservation of ω^n.

[2] It is also said that the flow of a Hamiltonian system is symplectic.

We conclude this section by putting the variational principle (2.6) in a form which will be useful later. Let us introduce in the phase space the new variables z^i, $i = 1, ..., 2n$, with $z^i = q_i$ and $z^{i+n} = p_i$, for $i = 1, \ldots, n$. We also define the quantities $\gamma_i = p_i$, $\gamma_{i+n} = 0$, $i = 1, \ldots, n$. Then, with these notations, (2.6) becomes

$$\delta \int dt(\gamma_i \frac{\partial}{\partial t} z^i - H(z, t)) = 0. \tag{2.10}$$

If we also set $z^0 = t$, $\gamma_0 = -H$, then 2.10 takes the very compact form

$$\delta \int \gamma_\mu dz^\mu = 0, \tag{2.11}$$

where the dot denotes the derivative with respect to time. Hamilton's equations are found by carrying out the variation in (2.11). Since the integrand of (2.11) is a scalar, if we change coordinates,

$$Z^\mu = Z^\mu(z), \tag{2.12}$$

then the new equations of motion are again obtained from (2.11). If the coordinate transformation is canonical, then the equations of motion in the new variables will be in Hamiltonian form. If the coordinate transformation is not canonical, the equations of motion obtained from (2.11) will not be in Hamiltonian form. Under the coordinate transformation (2.12) the 1-form $\gamma_\mu dz^\mu$ will become $\Gamma_\mu dZ^\mu$ and in general the components Γ_{n+i}, $i = 1, ..., n$ will not be zero. However, if the transformation is canonical then we will have $\Gamma_{n+i} = 0$, $i = 1, ..., n$. This can also be taken as a definition of canonical transformation: a canonical

transformation is a transformation (2.12) such that $\Gamma_{n+i} = 0$, $i = 1, ..., n$.

Let us now see how the equations for the magnetic field lines flow can be put into Hamiltonian form. Writing the magnetic field as $B = \nabla \wedge A$, then for the magnetic field lines we have the equations

$$(\nabla \wedge A) \wedge \frac{dx}{d\lambda} = 0, \tag{2.13}$$

where λ is an arbitrary parameter. If now we consider the variational principle (ref. [11])

$$\delta \int d\lambda A_\mu(x) dx^\mu / d\lambda = 0, \tag{2.14}$$

then, from the calculus of variations we know that we must have

$$\frac{d}{d\lambda}\frac{\partial g}{\partial \dot{x_k}} - \frac{\partial g}{\partial x_k} = 0, \tag{2.15}$$

where $g = A_\mu(x) dx^\mu / d\lambda$ and the dot denotes the derivative with respect to λ. We thus obtain

$$\frac{dA_k}{d\lambda} - \dot{x_\mu}\frac{\partial A_\mu}{\partial x_k} = 0, \tag{2.16}$$

which is the same as (2.13). We now perform a gauge transformation $A'_\mu = A_\mu + \partial_\mu S$ in order to eliminate one of the component of the vector potential, say the component A'_2. Then, we obtain (omitting the prime)

$$A_\mu dz^\mu = A_1 dz^1 + A_3 dz^3, \tag{2.17}$$

and, introducing the new variable $p = A_1(z^1, z^2, z^3)$ to replace z^2, we arrive at

$$A_\mu dz^\mu = p dz^1 + A_3(z^1, p, z^3) dz^3, \tag{2.18}$$

which has to be compared with (2.10). We see that $-A_3$ plays the role of the Hamiltonian for the magnetic field lines system and that z^1 and z^2 are canonically conjugate variables. The variable z^3 is the analogous of time. The variational principle (2.14) can also be written as

$$\delta \int A_\mu dz^\mu = 0, \tag{2.19}$$

which has the same form as (2.11). The field line flow is then obtained by applying Hamilton's equations to $-A_3$.

The vector γ_μ will be called 1-form (more precisely the 1-form is the quantity $\gamma_\mu dz^\mu$). The addition of the derivative of an arbitrary function S to the 1-form does not change the equations of motion obtained by carrying out the variation of (2.11), that is the 1-forms γ_μ and $\gamma_\mu + \partial_\mu S$ are equivalent.

2.3 The Lie Transform

In classical perturbation theory for Hamiltonian systems, in general a generating function F is used to perform a canonical transformation from the old variables q, p to the new variables Q, P. This generating function depends on both the old and the new variables, and as a consequence the transformation itself and the relation between the old Hamiltonian H and the new one K appear in a mixed form. For example, if the generating function is of the type $F(q, P, t)$, then for the coordinates we have the relations

$$Q(q, P, t) = \frac{\partial}{\partial P} F, \qquad p(q, P, t) = \frac{\partial}{\partial q} F, \tag{2.20}$$

and for the Hamiltonians

$$K(Q, P, t) = H(q, p, t) + \frac{\partial}{\partial t} F. \tag{2.21}$$

We see that (2.20) is in a mixed form, while what we actually need are the relations $Q(q, p, t)$ and $P(q, p, t)$, and that (2.21) is a relation between the functions H and K at corresponding points in phase space. When (2.20) and (2.21) are used as the basis for a perturbation analysis the result are very lengthy formulas even for very low orders. It would be preferable to have a formalism that yields directly the new variables in terms of the old one, or vice-versa, and such that the relation between H and K is a relation between functions.

This formalism has been developed by researchers working in celestial mechanics ([6], [7], [8], [9]), and has been presented in the review articles [10] and [11]. It is a formalism

based on the so called Lie transform, which is a special kind of coordinate transformation. The perturbation theory based on the Lie transform has a number of advantages. It is canonically invariant and it is possible to give a direct expansion of any function of the old variables in terms of the new variables. We present in this section a brief account of the perturbation theory based on the Lie transform. The great majority of the results are not derived, and the reader is referred especially to ref. [11] for a rigorous presentation of the theory.

Let us consider the coordinate transformation

$$Z^\mu = z^\mu + \epsilon Z_1^\mu(z) + \epsilon^2 Z_2^\mu(z) + \cdots, \tag{2.22}$$

from the variables $z^1, \ldots, z^n$, to the variables $Z^1, \ldots, Z^n$, where ϵ is a small parameter and $Z_1^\mu, Z_2^\mu, \ldots$ are functions of n variables. We will use the compact notation

$$Z^\mu = Z^\mu(z, \epsilon). \tag{2.23}$$

The transformation (2.23) is called a Lie transformation when the differential equation

$$\frac{\partial}{\partial \epsilon} Z^\mu = g^\mu(Z^\mu),$$

together with the initial condition $Z^\mu(z, 0) = z^\mu$, is satisfied by the functions Z^μ. The vector g^μ is called the generator of the Lie transform, and completely characterizes it.

Let us now see how coordinates and scalars transform under a Lie transform. We first introduce the operator L_g which maps scalar functions into scalar functions according to

$$L_g f = g^\mu \partial_\mu f. \tag{2.24}$$

Notice that this is a functional relationship, so the symbol for the independent variables is a dummy, and it could be z^μ or Z^μ or any other. It is then found that the old and the new coordinates are related by

$$z^\mu = e^{(-\epsilon L_g)} Z^\mu, \tag{2.25}$$

while a scalar $s(z)$ transforms in the opposite way, that is

$$S(Z) = e^{-\epsilon L_g} s(Z). \tag{2.26}$$

We will be particularly interested in the transformation properties of the expansion, according to a smallness parameter ϵ, of a 1-form

$$\gamma = \gamma^0 + \epsilon\gamma^1 + \epsilon^2\gamma^2 + \cdots, \tag{2.27}$$

which could represent, for instance, the magnetic vector potential or some other physical quantity. The superscript in the γ's indicate the order in ϵ. The 1-form (2.27) is better treated by a composition of individual Lie transforms, each of them characterized by its generator g^μ. In the following the lower index will represent the perturbative order, so that we will write g_n^μ to indicate the generators of the *nth* Lie transform, of order ϵ^n, and L_n will now indicate the operator such that, if σ is an arbitrary 1-form, then $(L_n\sigma)_\nu = g_n^\mu(\partial_\mu\sigma_\nu - \partial_\nu\sigma_\mu)$. [3] Notice that the convention is the opposite for the 1-form: for the 1-form the superscript represents the perturbative order. Our aim is to transform (2.27) into an

[3] We have shorten the notation by writing L_n instead of L_{g_n}.

expression of the form

$$\Gamma = \Gamma^0 + \epsilon\Gamma^1 + \epsilon^2\Gamma^2 + \cdots, \tag{2.28}$$

where Γ^1 is obtained by a Lie transform characterized by the generator g_1, Γ^2 is obtained by a Lie transform characterized by the generator g_2 and so on. It is found that γ and Γ are related by

$$\Gamma = T\gamma + dS, \tag{2.29}$$

where

$$T = \cdots T_3 T_2 T_1, \tag{2.30}$$

with

$$T_n = e^{-\epsilon^n L_{g_n}}, \tag{2.31}$$

and dS is a total differential which represents a gauge transformation of the 1-form and therefore does not affect the equations of motion. Expanding in powers of ϵ we obtain

$$\begin{aligned} \Gamma \;=\; & \cdots(1 - \epsilon^3 L_3 + \tfrac{1}{2}\epsilon^6 L_3^2 + \cdots) \\ & (1 - \epsilon^2 L_2 + \tfrac{1}{2}\epsilon^4 L_2^2 + \cdots) \\ & (1 - \epsilon L_1 + \tfrac{1}{2}\epsilon^2 L_1^2 + \cdots)\gamma + dS. \end{aligned} \tag{2.32}$$

Collecting the terms and using also the expansions for γ and Γ we obtain

$$\begin{aligned} \Gamma^0 &= \gamma^0, \\ \Gamma^1 &= dS_1 - L_1\gamma^0 + \gamma^1, \\ \Gamma^2 &= dS_2 - L_2\gamma^0 + \gamma^2 - L_1\gamma^1 + \tfrac{1}{2}L_1^2\gamma^0, \\ \Gamma^3 &= dS_3 - L_3\gamma^0 + \gamma^3 + L_2L_1\gamma^0 - \tfrac{1}{6}L_1^3\gamma^0 - L_2\gamma^1 + \tfrac{1}{2}L_1^2\gamma^1 - L_1\gamma^2, \end{aligned} \tag{2.33}$$

and so on. Here S represents a gauge function that will not alter the equations of motion. The coordinate transformation associated with the transformation of the 1-form is found observing that the coordinate transform controvariantly, that is

$$Z = T^{-1} z, \tag{2.34}$$

where

$$T^{-1} = T_1^{-1} T_2^{-1} T_3^{-1} \cdots, \tag{2.35}$$

with

$$T_n^{-1} = e^{\epsilon^n L_{gn}}. \tag{2.36}$$

Again, expanding and collecting the terms, we obtain

$$Z = z + \epsilon L_1 z + \epsilon^2 (\frac{1}{2} L_1^2 + L_2) z + \epsilon^3 (\frac{1}{6} L_1^3 + L_1 L_2 + L_3) z + \cdots. \tag{2.37}$$

To simplify the notation it is convenient to introduce the tensor ω, called Lagrange tensor, and defined by (ς is a 1-form)

$$\omega^{\varsigma}_{\mu\nu} = \partial_\mu \varsigma_\nu - \partial_\nu \varsigma_\mu, \tag{2.38}$$

so that we can write

$$(L_n \gamma^0)_\mu = g_n^\nu \omega^{\gamma^0}_{\nu\mu}. \tag{2.39}$$

When σ is one of the terms of (2.27), then we will further simplify the notation by writing $\omega^k_{\mu\nu}$ instead of $\omega^{\gamma^k}_{\mu\nu}$, so that, for example

$$\omega^0_{\mu\nu} = \partial_\nu \gamma^0_\mu - \partial_\mu \gamma^0_\nu. \tag{2.40}$$

The general form of Γ is therefore

$$\Gamma^n = dS_n - L_n \gamma^0 + C_n, \tag{2.41}$$

where C_n is a 1-form calculated from γ^n and the results of the preceding lower order calculations. The generator is contained in the term $L_n \gamma^0$. The expressions of C_1, C_2 and C_3 are

$$\begin{aligned} C_1 &= \gamma^1, \\ C_2 &= \gamma^2 - L_1 \gamma^1 + \tfrac{1}{2} L_1^2 \gamma^0 \\ C_3 &= L_2 L_1 \gamma^0 - \tfrac{1}{6} L_1^3 \gamma^0 - L_2 \gamma^1 + \tfrac{1}{2} L_1^2 \gamma^1 - L_1 \gamma^2. \end{aligned} \tag{2.42}$$

It is possible to choose $g_n^0 = 0$ to all orders, and this corresponds to the fact that usually we do not want to transform also the time when we change coordinates. The 2N components g_n^i and the scalar S_n can be chosen as to bring the 2N + 1 components of Γ^n, where N is the number of degrees of freedom, into some desired form. We want a form in which only the temporal component of Γ, which will be the φ-component in our case, is not zero, and this can be done choosing

$$g_n^j = (\partial_i S_n + C_{ni}) J_0^{ij}, \tag{2.43}$$

where J_0^{ij} is the inverse of the spatial part of the Lagrange tensor. With this choice of the generators the temporal component of the 1-form becomes

$$\Gamma_t^n = V_0^\mu \partial_\mu S_n + C_{n\mu} V_0^\mu, \tag{2.44}$$

where V_0^μ is the Poisson vector, defined as $V_0^i = J_0^{ij} \omega^0_{0j}$, $V_0^0 = 1$. We stress that with the

choice (2.43) of the generators, the temporal component of the 1- form is the only one which survives after the transformation.

Chapter 3

Magnetic Field Lines Hamiltonian

3.1 Introduction

In this chapter we discuss Hamiltonian formulations for the magnetic field lines system. We first use a gauge transformation to eliminate the component ψ of the vector potential and then expand the non vanishing components in Taylor series. Then we apply perturbation theory based on the Lie transform to transform systematically to canonical variables. In section 3.4 we show the procedure rather in detail for the cylindrical limit approximation of the field. In section 3.5 we derive a Hamiltonian correct until the third perturbative order for the toroidal helical case, and in the following section we discuss a different Hamiltonian.

3.2 Magnetic Potential

The general scalar potential satisfying the condition $\nabla^2\Psi = 0$, regular at $\xi = 0$, and allowing for an axial current is (refs. [12], [13])

$$\Psi = I\varphi + (1-\xi\cos\eta)^{1/2} \sum_{l,m=-\infty}^{+\infty} \alpha_{lm} U_{lm}(\xi) e^{il\eta+im\varphi}, \tag{3.1}$$

where

$$U_{lm}(\xi) = \xi^{-1/2} Q^{|m|}_{l-\frac{1}{2}}(1/\xi). \tag{3.2}$$

The coordinates ξ, η and φ are toroidal coordinates, in terms of which the Cartesian coordinates are $z = \xi\sin\eta/(1-\xi\cos\eta)$, $x = (1-\xi^2)^{1/2}\cos\varphi/(1-\xi\cos\eta)$, and $y = (1-\xi^2)^{1/2}\sin\varphi/(1-\xi\cos\eta)$. Units are selected such that $I = 1$. The coefficients α_{lm} are arbitrary provided that $\alpha_{lm} = \alpha^*_{-(lm)}$. The function Q^μ_ν is the modified Legendre function of second kind. From the potential Ψ the component for the vector potential for the divergence-free and curl-free magnetic field are obtained as explained in ref. [13] and the vector potential can be written as

$$A = (\sum_{l,m} \alpha_{lm} A^{lm}_\xi, A^T_\eta + \sum_{l,m} \alpha_{lm} A^{lm}_\eta, \sum_l \alpha_{l0} A^{l0}_\varphi), \tag{3.3}$$

where

$$A^T_\eta = (1/2)[(1-\cos\eta)^{-1}\ln(\frac{1-\xi\cos\eta}{1-\xi}) + (1-\cos\eta)^{-1}\ln(\frac{1-\xi\cos\eta}{1+\xi})], \tag{3.4}$$

$$A^{lm}_\xi = \frac{-i}{m\xi(1-\xi\cos\eta)} U_{lm}(\xi)\partial_\eta(1-\xi\cos\eta)^{1/2} e^{il\eta+im\varphi}, \tag{3.5}$$

$$A_\eta^{lm} = \frac{i}{m(1-\xi\cos\eta)}\xi(1-\xi^2)\partial_\xi(1-\xi\cos\eta)^{1/2}U_{lm}(\xi)e^{il\eta+im\varphi}, \tag{3.6}$$

$$A_\varphi^{l0} = -\int_0^\xi dx[x(1-x\cos\eta)]^{-1}U_{l0}(x)\partial_\eta(1-x\cos\eta)^{1/2}e^{il\eta}. \tag{3.7}$$

We select the harmonics (l,m) and $(l,0)$, that is we will consider the potential

$$A = (\epsilon A_\xi^{lm}, A_\eta^T + \epsilon A_\eta^{lm}, \epsilon' A_\varphi^{l0}), \tag{3.8}$$

where $\epsilon = \alpha_{lm}, \epsilon' = \alpha_{l0}$. Now, in order to apply the Lie transform, we consider the 1-form

$$\gamma = (\epsilon A_\xi^{lm} + \partial_\xi S)d\xi + (A_\eta^T + \epsilon A_\eta^{lm} + \partial_\eta S)d\eta + (\epsilon' A_\varphi^{l0} + \partial_\varphi S)d\varphi, \tag{3.9}$$

where S is a gauge function. Exploiting the gauge freedom, we choose the gauge function in order to make the ξ component of the 1-form to vanish, that is we choose the gauge function to be

$$S = -\epsilon\int d\xi A_\xi^{lm}, \tag{3.10}$$

and therefore the 1-form becomes

$$\gamma = (A_\eta^T + \epsilon A_\eta^{lm} - \epsilon\int d\xi\partial_\eta A_\xi^{lm})d\eta + (\epsilon' A_\varphi^{l0} - \epsilon\int d\xi\partial_\varphi A_\xi^{lm})d\varphi. \tag{3.11}$$

We now introduce the new variable $\theta = \eta + (m/l)\varphi$, where l is the poloidal multipolarity and m is the number of field periods, so that we obtain

$$\begin{aligned}\gamma &= [A_\eta^T + \epsilon A_\eta^{lm} - \epsilon\int d\xi\partial_\eta A_\eta^{lm}]d\theta \\ &\quad +[\epsilon' A_\varphi^{l0} - (m/l)(A_\eta^T + \epsilon A_\eta^{lm}) \\ &\quad -\epsilon\int d\xi(\partial_\varphi A_\xi^{lm} - (m/l)\partial_\eta A_\xi^{lm})]d\varphi.\end{aligned} \tag{3.12}$$

The 1-form is of the type $\gamma = \gamma_\theta d\theta + \gamma_\varphi d\varphi$, where

$$\gamma_\theta = A_\eta^T + \epsilon A_\eta^{lm} - \epsilon\int d\xi\partial_\eta A_\eta^{lm}, \tag{3.13}$$

and

$$\begin{aligned}\gamma_\varphi &= \epsilon' A_\varphi^{l0} - (m/l)(A_\eta^T + \epsilon A_\eta^{lm}) - \epsilon\int d\xi(\partial_\varphi A_\xi^{lm} - (m/l)\partial_\eta A_\xi^{lm}) \\ &= \epsilon' A_\varphi^{l0} - (m/l)\gamma_\theta - \epsilon\int d\xi\partial_\varphi A_\xi^{lm}.\end{aligned} \tag{3.14}$$

In the next section we will expand the 1-form in Taylor series in the variable ξ.

3.3 Taylor Expansion of the Potential

To apply the Lie transformation we need to have the 1-form written as an expansion of the type (2.27). We will consider ϵ, ϵ' and ξ as smallness parameters of the same order, and we will expand the 1-form in the variable ξ about the point $\xi = 0$. We proceed first to the expansion of the quantities $U_{lm}(\xi)$. The functions $U_{lm}(\xi)$ admit the integral representation (ref. [13])

$$U_{lm}(\xi) = \beta_{lm}\xi^l(1-\xi^2)^{-m/2}\int_0^\pi dt(\sin t)^{2l}(1+\xi\cos t)^{m-l-1/2}. \tag{3.15}$$

Expanding $(1-\xi^2)^{-m/2}$ and $(1+\xi\cos t)^{m-l-1/2}$, we can put (3.15) in the form

$$U_{lm}(\xi) = \xi^l(U_{lm}^0 + \xi U_{lm}^1 + \xi^2 U_{lm}^2 + \cdots), \tag{3.16}$$

where the normalization constants β_{lm} have been incorporated into the constant quantities $U^0_{2m}, U^1_{2m}, \ldots$. From now on we will set $l = 2$. For the other terms we obtain

$$
\begin{aligned}
A^T_\eta &= (1/2)\xi^2 + (1/3)\xi^3 \cos\eta + (1/4)\xi^4(1+\cos\eta^2) + \cdots, \\
A^{2m}_\eta &= (2i/m)U^0_{2m}\xi^2 e^{2i\theta} + \\
&\quad (i/2m)\cos\eta U^0_{2m}\xi^3 e^{2i\theta} + \\
&\quad (i/m)(2U^{2\ 2}_{2m} - U^0_{2m})\xi^4 e^{2i\theta} + \cdots, \\
A^{2m}_\xi &= (2/m)U^0_{2m}\xi e^{2i\theta} + \\
&\quad (1/2m)U^0_{2m}(2\cos\eta - \sin\eta)\xi^2 e^{2i\theta} + \cdots, \\
A^{20}_\varphi &= -iU^0_{20}\xi^2 e^{2i\eta} - \\
&\quad (1/6)U^0_{20}(\sin\eta + 2i\cos\eta)\xi^3 e^{2i\eta} + \cdots.
\end{aligned}
\tag{3.17}
$$

The quantities U^i_{lm} are constant, and the only values that we will need are $U^0_{20} = 1/2$, $U^0_{2m} = (m^2)/8$, $U^1_{20} = 0$, $U^1_{2m} = 0$ and $U^2_{20} = 35/96$. Putting all the terms together, introducing the new variable $\psi = (1/2)\xi^2$ and taking the real part of the various terms in

(3.17) we obtain, up to the third order, the following expansion for γ_θ

$$
\begin{aligned}
\gamma^0_\theta &= \psi, \\
\gamma^1_\theta &= (1/3)(2\psi)^{3/2}\cos((m\varphi)/2 - \theta), \\
\gamma^2_\theta &= \psi^2(1 + \cos((m\varphi)/2 - \theta)^2), \\
\gamma^3_\theta &= (1/5)\sqrt{2}\psi^{5/2}(7\cos((m\varphi)/2 - \theta) + \cos((3m\varphi)/2 - 3\theta) + \\
&\quad (1/(4m))\epsilon\,\psi^2\,(35\,U^0_{2m} - 48\,U^2_{2m})\,\sin(2\theta),
\end{aligned}
\tag{3.18}
$$

and for γ_φ

$$
\begin{aligned}
\gamma^0_\varphi &= -(m\psi)/2, \\
\gamma^1_\varphi &= -(1/3)\sqrt{2}m\psi^{3/2}\cos((m\varphi)/2 - \theta) - \\
&\quad 2\,\epsilon'\,\psi\,U^0_{20}\,\sin(m\,\varphi - 2\,\theta) + 2\,\epsilon\,\psi\,U^0_{2m}\,\sin(2\,\theta), \\
\gamma^2_\varphi &= -(3/4)m\psi^2 - (1/4)m\psi^2\cos(m\,\varphi - 2\,\theta) - \\
&\quad (3\sqrt{2})^{-1}\epsilon\psi^{3/2}U^0_{2m}\sin((m\varphi)/2 - 3\theta) - (3\sqrt{2})^{-1}\epsilon'\psi^{3/2}U^0_{20}\sin((3m\varphi)/2 - 3\theta) - \\
&\quad (1/\sqrt{2})\epsilon'\psi^{3/2}U^0_{20}\sin((m\varphi)/2 - \theta) + (1/\sqrt{2})\epsilon\psi^{3/2}U^0_{2m}\sin((m\varphi)/2 + \theta), \\
\gamma^3_\varphi &= -(1/(5\sqrt{2}))m\psi^{5/2}\cos((3m\varphi)/2 - 3\theta) - ((7m)/(5\sqrt{2}))\psi^{5/2}\cos((m\varphi)/2 - \theta) + \\
&\quad (3/8)\,\epsilon\,\psi^2\,U^0_{2m}\,\sin(m\,\varphi) - (3/8)\,\epsilon'\,\psi^2\,U^0_{20}\,\sin(m\,\varphi - 2\,\theta) - \\
&\quad 2\,\epsilon'\,\psi^2\,U^2_{20}\,\sin(m\,\varphi - 2\,\theta) - 4\,\epsilon\,\psi^2\,U^0_{2m}\,\sin(2\,\theta) + 8\,\epsilon\,\psi^2\,U^2_{2m}\,\sin(2\,\theta).
\end{aligned}
\tag{3.19}
$$

3.4 Cylindrical Limit Approximation

In this section we apply the Lie transform technique to the cylindrical limit approximation of the magnetic field, which is the approximation that neglects the toroidicity of the field. The field becomes therefore a straight helical field. The calculations will be carried out in great detail in order to illustrate with a simple example the use of the Lie transform. The calculation scheme described below will be used, unchanged, when we will take into account also the toroidicity of the field. In the case of the cylindrical limit approximation we have

$$A_\eta^T = \frac{\xi^2}{2}, \tag{3.20}$$

$$A_\xi^{lm} = \frac{l}{m\xi} I_l(m\xi) e^{il\eta + im\varphi}, \tag{3.21}$$

$$A_\eta^{lm} = \frac{i\xi}{m} \partial_\xi I_l(m\xi) e^{il\eta + im\varphi}, \tag{3.22}$$

$$A_\varphi^{l0} = 0. \tag{3.23}$$

The $I_l(m\xi)$ are the modified Bessel functions, that is solutions of the equation

$$\partial_\xi(\xi \partial_\xi W) = (\frac{l^2}{\xi} + m^2\xi) W, \tag{3.24}$$

and they admit the series expansion

$$\begin{aligned} I_l(m\xi) &= (\tfrac{m\xi}{2})^2 \textstyle\sum_{k=0}^{k=\infty} \frac{(\frac{m\xi}{2})^{2k}}{k!\Gamma(k+l+1)} \\ &= \xi^2 (I_l^{(0)} + \xi^2 I_{(l)}^2 + \xi^4 I_{(l)}^2 + \cdots, \end{aligned} \tag{3.25}$$

and, for $l = 2$, we have for the first two terms

$$I_2^{(0)} = \frac{1}{2!}(\frac{m}{2})^2, \tag{3.26}$$

$$I_2^{(2)} = \frac{1}{3!}(\frac{m}{2})^4. \tag{3.27}$$

For the cylindrical limit case it is convenient to use the formula

$$\begin{aligned} \gamma &= [A_\eta^T + \epsilon A_\eta^{lm} - \epsilon \int d\xi \partial_\eta A_\eta^{lm}] d\theta \\ &\quad + [\epsilon' A_\varphi^{l0} - (m/l)(A_\eta^T + \epsilon A_\eta^{lm}) \\ &\quad - \epsilon \int d\xi (\partial_\varphi A_\xi^{lm} - (m/l)\partial_\eta A_\xi^{lm})] d\varphi, \end{aligned} \tag{3.28}$$

and observe that $\partial_\varphi A_\xi^{lm} - (m/l)\partial_\eta A_\xi^{lm} = 0$. Then, expanding the quantities A_η^T, A_η^{lm}, A_ξ^{lm} in Taylor series about the point $\xi = 0$, taking the real parts and introducing the variables $\psi = (1/2)\xi^2$ and $\theta = \eta + (m/l)\varphi$, we obtain

$$\begin{aligned} &\gamma_\theta^0 = \psi, && \gamma_\varphi^0 = -(m/2)\psi, \\ &\gamma_\theta^1 = 0, && \gamma_\varphi^1 = \epsilon\psi(m^2/4)\sin(2\theta), \\ &\gamma_\theta^2 = -\epsilon(m^3/8)\psi^2 \sin(2\theta), && \gamma_\varphi^2 = \epsilon(m^4/12)\psi^2 \sin(2\theta). \end{aligned} \tag{3.29}$$

From the expansion above we see that the lowest order part of the vector potential is

$$\gamma^0 = \psi d\theta - (m/2)\psi d\varphi. \tag{3.30}$$

This expression is already in canonical form, θ and φ play the role of canonical conjugate variables and the unperturbed Hamiltonian is $H = (m/2)\psi$. Actually it was the introduction of the variable $\psi = (1/2)\xi^2$ that put the lowest order potential in canonical form. The

lowest order of the vector potential, and the corresponding Hamiltonian $H = (m/2)\psi$ will be considered the unperturbed part of the potential.

We now recall, for convenience, the formulas for the generators of the Lie transform and for the temporal part of the transformed 1-form. We have (see eqs. (2.43) and (2.44))

$$g_n^j = (\partial_i S_n + C_{ni}) J_0^{ij}, \tag{3.31}$$

$$\Gamma_t^n = V_0^\mu \partial_\mu S_n + C_{n\mu} V_0^\mu, \tag{3.32}$$

where J_0^{ij} is the inverse of the spatial part of the Lagrange tensor and V_0^μ is the Poisson vector, defined as $V_0^i = J_0^{ij}\omega_{0j}^0$, $V_0^0 = 1$. In our calculations we have three variables: φ, θ and ψ. The variable φ corresponds to the time, and therefore the temporal part of the 1-form is the one corresponding to φ. Let us now see how eqs. (3.31) and (3.32) appear in our case. First we note that the zeroth component of the transformed 1-form is equal to the unperturbed one, that is

$$\Gamma^0 = \psi d\theta - (m/2)\psi d\varphi. \tag{3.33}$$

We use this expression to calculate the Lagrange tensor ω^0, the inverse of its spatial part J_0^{ij} and the Poisson vector V_0^μ. For the Lagrange tensor we obtain

$$\omega_{\varphi\theta}^0 = \partial_\varphi \gamma_\theta^0 - \partial_\theta \gamma_\varphi^0 = 0, \tag{3.34}$$

$$\omega_{\varphi\psi}^0 = \partial_\varphi \gamma_\psi^0 - \partial_\psi \gamma_\varphi^0 = m/2, \tag{3.35}$$

$$\omega_{\theta\psi}^0 = \partial_\theta \gamma_\psi^0 - \partial_\psi \gamma_\theta^0 = -1. \tag{3.36}$$

The Lagrange tensor is therefore the 3-dimensional matrix

$$\begin{pmatrix} 0 & 0 & m/2 \\ 0 & 0 & -1 \\ -m/2 & 1 & 0 \end{pmatrix},$$

and its spatial part is

$$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix},$$

from which we obtain its inverse, the matrix J_0^{ij}

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

The Poisson vector is now obtained from the formula $V_0^j = J_0^{ij}\omega_{0j}^0$. Accordingly

$$V_0^\psi = 0, \qquad V_0^\theta = m/2, \tag{3.37}$$

and we remind the reader that by definition $V_0^\varphi = 1$. Using these results, from eq. (3.31) we obtain

$$g_n^\theta = -\partial_\psi S_n - C_{n\psi}, \tag{3.38}$$

$$g_n^\psi = \partial_\theta S_n + C_{n\theta}, \tag{3.39}$$

and $g_n^\varphi = 0$ for every n. The expression (3.32) for Γ_φ^n is given by

$$\Gamma_\varphi^n = \partial_\varphi S_n + V_0^\psi \partial_\psi S_n + V_0^\theta \partial_\theta S_n + C_{n\varphi} + V_0^\psi C_{n\psi} + V_0^\theta C_{n\theta}, \tag{3.40}$$

and substituting the Poisson vector, we obtain

$$\Gamma^n_\varphi = \partial_\varphi S_n + (m/2)\partial_\theta S_n + C_{n\varphi} + (m/2)C_{n\theta}. \tag{3.41}$$

We see that, for every order n, the basic formulas (3.38), (3.39) and (3.41) suggest two possible strategies:

1) first we choose the generators. Then (3.38) and (3.39) give us the equations by which we determine the gauge function S. Substituting in (3.41) we obtain the transformed 1-form.

2) first we choose the gauge function S, then from (3.38), (3.39) and (3.41) we obtain the generators and the transformed 1-form.

The two strategies are completely equivalent, and using one or the other is a matter of choice. We will proceed according to 2), because choosing first the gauge function allows one to specify more directly the form of the transformed 1-form. A typical choice would be to choose S_n such that the equation

$$< \partial_\varphi S_n + (m/2)\partial_\theta S_n >= 0, \tag{3.42}$$

where the brackets denote average, is satisfied. This corresponds to taking Γ^n as the average of $C_{n\varphi} + (m/2)C_{n\theta}$ over the same variables as (3.42).

Finally, we stress that (3.38), (3.39) and (3.41) are derived under the requirement that only the temporal part of Γ, that is Γ^φ, is not zero after the Lie transformation of coordinates.

We now proceed to the calculation of the first order contribution to Γ^0. We start by taking Γ^1_φ as the average over θ of the quantity $V_0^\mu C_{1\mu} = \gamma^1_\varphi + (m/2)\gamma^1_\theta$, which vanishes, since

$$\gamma^1_\varphi + (m/2)\gamma^1_\theta = \epsilon(m^2/4)\psi \sin 2\theta. \tag{3.43}$$

We have now to calculate the first order gauge function and the first order Lie generators, which will be necessary in order to calculate the second order component of the transformed 1-form. To calculate the first order gauge function, we have to solve the equation

$$\partial_\varphi S_1 + (m/2)\partial_\theta S_1 = -\gamma^1_\varphi - (m/2)\gamma^1_\theta. \tag{3.44}$$

A solution of this equation is a gauge function which does not depend on φ, that is

$$S_1 = (1/4)\epsilon\psi \cos 2\theta. \tag{3.45}$$

The generators are obtained from eqs. (3.38) and (3.39) which explicitly read

$$g^\theta_1 = -\partial_\psi S_1 = -(1/4)\epsilon m \cos 2\theta, \tag{3.46}$$

$$g^\psi_1 = \partial_\theta S_1 + \gamma^1_\theta = -(1/2)\epsilon m\psi \sin 2\theta. \tag{3.47}$$

At the first order we see therefore that there is no contribution to the unperturbed Hamiltonian. Let us proceed to the second order calculations. From (3.41) we obtain

$$\Gamma^2_\varphi = \partial_\varphi S_2 + (m/2)\partial_\theta S_2 + C_{2\varphi} + (m/2)C_{2\theta}, \tag{3.48}$$

and therefore we now have to evaluate the θ and φ components of the quantity

$$C_2 = \gamma^2 - L_1\gamma^1 + (1/2)L_1^2\gamma^0. \tag{3.49}$$

We have

$$\begin{aligned}(L_1\gamma^1)_\theta &= g_1^\psi \omega^1_{\psi\theta} \\ &= g_1^\psi \partial_\psi \gamma^1_\theta = 0,\end{aligned} \tag{3.50}$$

$$\begin{aligned}(L_1\gamma^1)_\varphi &= g_1^\theta \omega^1_{\theta\varphi} + g_1^\psi \omega^1_{\psi\varphi} \\ &= g_1^\psi \partial_\psi \gamma^1_\varphi + g_1^\theta \partial_\theta \gamma^1_\varphi \\ &= -(1/8)\epsilon^2 m^3 \psi.\end{aligned} \tag{3.51}$$

Besides, we have

$$\begin{aligned}(L_1^2\gamma^0)_\theta &= g_1^\psi \omega^{L_1\gamma^0}_{\psi\theta} \\ &= g_1^\psi [\partial_\psi (L_1\gamma^0)_\theta - \partial_\theta (L_1\gamma^0)_\psi],\end{aligned} \tag{3.52}$$

$$\begin{aligned}(L_1^2\gamma^0)_\varphi &= g_1^\theta \omega^{L_1\gamma^0}_{\theta\varphi} + g_1^\psi \omega^{L_1\gamma^0}_{\psi\varphi} \\ &= g_1^\theta [\partial_\theta (L_1\gamma^0)_\varphi - \partial_\psi (L_1\gamma^0)_\theta] \\ &\quad + g_1^\psi [\partial_\psi (L_1\gamma^0)_\varphi - \partial_\varphi (L_1\gamma^0)_\psi],\end{aligned} \tag{3.53}$$

and therefore we have to calculate first the components of the operator $L_1\gamma^0$. We obtain

$$(L_1\gamma^0)_\theta = g_1^\psi \omega^0_{\psi\theta} = -(1/2)\epsilon m \psi \sin 2\theta, \tag{3.54}$$

$$(L_1\gamma^0)_\psi = g_1^\theta \omega^0_{\theta\psi} = (1/4)\epsilon m \cos 2\theta, \tag{3.55}$$

$$(L_1\gamma^0)_\varphi = g_1^\theta \omega^0_{\theta\varphi} + g_1^\psi \omega^0_{\psi\theta} = (1/4)m^2 \epsilon \psi \sin 2\theta. \tag{3.56}$$

Substituting these relations into (3.52) and (3.53) we obtain

$$(1/2)(L_1^2\gamma^0)_\theta = 0, \tag{3.57}$$

$$(1/2)(L_1^2\gamma^0)_\varphi = -(1/16)\epsilon^2 m^3 \psi. \tag{3.58}$$

Using these results we obtain

$$C_{2\theta} = \gamma^2_\theta - (L_1\gamma^1)_\theta + (1/2)(L_1^2\gamma^0)_\theta = -(1/8)\epsilon m^3 \psi^2 \sin 2\theta, \tag{3.59}$$

$$\begin{aligned}C_{2\varphi} &= \gamma^2_\varphi - (L_1\gamma^1)_\psi + (1/2)(L_1^2\gamma^0)_\varphi \\ &= (1/12)\epsilon m^4 \psi^2 \sin 2\theta + (1/8)\epsilon^2 m^3 \psi - (1/16)\epsilon^2 m^3 \psi \\ &= (1/12)\epsilon m^4 \psi^2 \sin 2\theta + (1/16)\epsilon^2 m^3 \psi.\end{aligned} \tag{3.60}$$

Averaging over θ the quantity

$$C_{2\varphi} + (m/2)C_{2\theta}, \tag{3.61}$$

we obtain the second order contribution to the transformed 1-form

$$\Gamma^2_\varphi = (1/16)\epsilon^2 m^3 \psi. \tag{3.62}$$

Accordingly, the expression of the transformed 1-form up to the second order is

$$\Gamma = \psi d\theta + [-(m/2)\psi + (1/16)\epsilon^2 m^3 \psi] d\varphi. \tag{3.63}$$

In this expression the magnetic potential is expressed in canonical form, with ψ and θ playing the role of action angle variables. The Hamiltonian up to the second order is

$$H = (m/2)\psi - (1/16)\epsilon^2 m^3 \psi. \tag{3.64}$$

The equations of the magnetic field lines flow are obtained directly from the above expression. This result is consistent with the result obtained in ref. [2].

3.5 Helical Toroidal Potential

We now proceed to the calculation of the transformed 1-form in the toroidal case, along the same line followed for the cylindrical limit approximation. The starting point is again the expansion of the magnetic potential, which we report for convenience until the first order

$$\begin{aligned} \gamma_\theta^0 &= \psi, \\ \gamma_\theta^1 &= (1/3)(2\psi)^{3/2} \cos((m\varphi)/2 - \theta), \end{aligned} \tag{3.65}$$

$$\begin{aligned} \gamma_\varphi^0 &= -(m\psi)/2, \\ \gamma_\varphi^1 &= -(1/3)\sqrt{2} m \psi^{3/2} \cos((m\varphi)/2 - \theta) - \\ & 2\,\epsilon'\,\psi\,U_{20}^0\,\sin(m\,\varphi - 2\,\theta) + 2\,\epsilon\,\psi\,U_{2m}^0\,\sin(2\,\theta). \end{aligned} \tag{3.66}$$

We note that the zeroth order term is equal to the zeroth order term of the cylindrical limit approximation. The zeroth order in the expansion is the unperturbed part of the potential

$$\gamma^0 = \psi d\theta - \frac{m}{2}\psi d\varphi, \tag{3.67}$$

and it is in canonical form, with θ and ψ playing the role of action angle variables and $-\gamma_\varphi^0$ playing the role of the Hamiltonian for the unperturbed system. We now proceed to the calculations of the transformed 1-form to the various perturbative orders. For the zeroth order we have that the 1-form is left unchanged, that is

$$\Gamma^0 = \gamma^0 = \psi d\theta - (m/2)\psi d\varphi. \tag{3.68}$$

We also note that this is the same expression that we obtained in the cylindrical limit approximation, therefore the Lagrange tensor ω^0, the Poisson vector V^μ and the tensor J_0^{ij} are the same as for the cylindrical limit approximation of the field, that is we have

$$\omega^0_{\varphi\theta} = 0, \quad \omega^0_{\varphi\psi} = m/2, \quad \omega^0_{\theta\psi} = -1, \tag{3.69}$$

and

$$V_0^\psi = 0, \quad V_0^\theta = m/2, \quad V_0^\varphi = 1. \tag{3.70}$$

This means that eqs. (3.41), (3.38) and (3.39) are left unchanged, and therefore for the first order transformed 1-form we have to calculate the expression

$$\Gamma^1_\varphi = \partial_\varphi S_1 + (m/2)\partial_\theta S_1 + \gamma^1_\varphi + (m/2)\gamma^1_\theta. \tag{3.71}$$

In the above equation we can choose the gauge function to be zero, so that the expression for Γ^1_φ becomes

$$\Gamma^1_\varphi = \gamma^1_\varphi + (m/2)\gamma^1_\theta, \tag{3.72}$$

and, using the Taylor expansion for γ we obtain

$$\Gamma^1_\varphi = -2\psi\epsilon' U^0_{20}\sin(m\varphi - 2\theta) + \epsilon U^0_{2m}\sin(2\theta). \tag{3.73}$$

For the first order generators we have

$$g_1^\theta = -\partial_\psi S_1 - C_{1\psi}, \tag{3.74}$$

$$g_1^\psi = \partial_\theta S_1 + C_{1\theta}. \tag{3.75}$$

Since $S_1 = 0$ and $C_{1\psi} = 0$ we obtain

$$g_1^\theta = 0, \tag{3.76}$$

$$g_1^\psi = 2^{3/2}/3\psi^{3/2}\cos(m/2\varphi - \theta). \tag{3.77}$$

The equation for the second order contribution is

$$\Gamma^2_\varphi = \partial_\varphi S_2 + V_0^\theta\partial_\theta S_2 + V_0^\psi\partial_\psi S_2 + C_{2\varphi} + C_{2\theta}V_0^\theta + C_{2\psi}V_0^\psi, \tag{3.78}$$

which becomes, after substituting the values of the Poisson vector

$$\Gamma^2_\varphi = \partial_\psi S_2 + (m/2)\partial_\theta S_2 + C_{2\varphi} + (m/2)C_{2\theta}. \tag{3.79}$$

For the second order we need therefore to evaluate the quantity $C_2 = \gamma^2 - L_1\gamma^1 + (1/2)L_1^2\gamma^0$. The calculations of the explicit expression of the operators L's are straightforward but the algebra is quite lengthy, so we give only the results

$$\begin{aligned}(L_1\gamma^1)_\varphi &= -(2^{1/2}/3)\psi^{3/2}\cos(m/2\varphi - \theta)\times \\ &\quad (2^{1/2}m\psi^{1/2}\cos(m/2\varphi - \theta) + 4\epsilon U^0_{20}\sin(m\varphi - 2\theta) - \\ &\quad 4\epsilon' U^0_{2m}\sin(2\theta)),\end{aligned} \tag{3.80}$$

$$(L_1\gamma^1)_\theta = (4/3)\psi^2\cos((m/2)\varphi - \theta)^2, \tag{3.81}$$

$$(1/2)(L_1^2\gamma^0)_\varphi = -(2/3)m\psi^2\cos((m/2)\varphi-\theta)^2, \tag{3.82}$$

$$(1/2)(L_1^2\gamma^0)_\theta = (4/3)m\psi^2\cos((m/2)\varphi-\theta)^2. \tag{3.83}$$

The equation for Γ^2_φ is

$$\Gamma^2_\varphi = \partial_\varphi S_2 + (m/2)\partial_\theta S_2 + C_{2\varphi} + (m/2)C_{2\theta}, \tag{3.84}$$

and, choosing again the second order gauge function to vanish, we obtain

$$\begin{aligned}\Gamma^2_\varphi &= 2^{-1/2}\epsilon U^0_{2m}\sin(m/2\varphi-3\theta) + (1/(3\sqrt{2}))\epsilon\psi^{3/2}U^0_{20}\sin(m/2\varphi-\theta) + \\ &\quad 2^{-1/2}\epsilon'\psi^{3/2}U^0_{20}\sin(3/2m\varphi-3\theta) + \\ &\quad (1/(3\sqrt{2}))\epsilon\psi^{3/2}U^0_{2m}\sin(m/2\varphi+\theta).\end{aligned} \tag{3.85}$$

For the second order generators we obtain from eq. (2.43)

$$g_2^\theta = -\partial_\psi S_2 - C_{2\psi}, \tag{3.86}$$

$$g_2^\psi = \partial_\theta S_2 + C_{2\theta}. \tag{3.87}$$

Since $S_2 = 0$ and $C_{2\psi} = 0$ we obtain

$$g_2^\theta = 0, \tag{3.88}$$

$$g_2^\psi = (1/6)\psi^2(7+\cos(m\varphi-2\theta)). \tag{3.89}$$

To proceed to the calculations of the third order we have to calculate now the quantity

$$C_3 = L_2L_1\gamma^0 - (1/6)L_1^3\gamma^0 - L_2\gamma^1 + (1/2)L_1^2\gamma^1 - L_1\gamma^2. \tag{3.90}$$

Calculating the above expression and choosing again the gauge function to vanish, we find for Γ^3 the following expression

$$\begin{aligned}\Gamma^3 &= (1/24)\epsilon\psi^2U^0_{2m}\sin(m\varphi) + (47/24)\epsilon'\psi^2U^0_{20}\sin(m\varphi-2\theta) - \\ &\quad (47/24)\epsilon\psi^2U^0_{2m}\sin(2\theta) - 2\epsilon'\psi^2U^2_{20}\sin(m\varphi-2\theta) + \\ &\quad 2\epsilon\psi^2U^2_{2m}\sin(2\theta).\end{aligned} \tag{3.91}$$

Up to the third order the Hamiltonian is given by

$$H = -\Gamma_\varphi = -\Gamma^0_\varphi - \Gamma^1_\varphi - \Gamma^2_\varphi - \Gamma^3_\varphi. \tag{3.92}$$

For convenience we collect below the various contributions.

$$H_0 = \frac{m\,\psi}{2}, \tag{3.93}$$

$$H_1 = 2\,\epsilon'\,\psi\,U^0_{20}\,\sin(m\,\varphi-2\,\theta) - 2\,\epsilon\,\psi\,U^0_{2m}\,\sin(2\,\theta), \tag{3.94}$$

$$\begin{aligned}H_2 &= -\frac{\epsilon\,\psi^{\frac{3}{2}}\,U^0_{2m}\,\sin(\frac{m\,\varphi}{2}-3\,\theta)}{\sqrt{2}} - \frac{\epsilon'\,\psi^{\frac{3}{2}}\,U^0_{20}\,\sin(\frac{3\,m\,\varphi}{2}-3\,\theta)}{\sqrt{2}} - \\ &\quad \frac{\epsilon'\,\psi^{\frac{3}{2}}\,U^0_{20}\,\sin(\frac{m\,\varphi}{2}-\theta)}{3\,\sqrt{2}} + \frac{\epsilon\,\psi^{\frac{3}{2}}\,U^0_{2m}\,\sin(\frac{m\,\varphi}{2}+\theta)}{3\,\sqrt{2}},\end{aligned} \tag{3.95}$$

$$\begin{aligned}H_3 &= \frac{-(\epsilon\,\psi^2\,U^0_{2m}\,\sin(m\,\varphi))}{24} - \frac{47\,\epsilon'\,\psi^2\,U^0_{20}\,\sin(m\,\varphi-2\,\theta)}{24} + \\ &\quad 2\,\epsilon'\,\psi^2\,U^2_{20}\,\sin(m\,\varphi-2\,\theta) + \frac{47\,\epsilon\,\psi^2\,U^0_{2m}\,\sin(2\,\theta)}{24} - 2\,\epsilon\,\psi^2\,U^2_{2m}\,\sin(2\,\theta).\end{aligned} \tag{3.96}$$

3.6 Integrable Model

In this section we discuss a different Hamiltonian for the toroidal helical magnetic field. We observe that the perturbation theory based on the Lie transform allows a certain freedom of choice in selecting the transformed variables. In fact it can be noticed from eq. (3.41) that choosing a different gauge function would lead to different Hamiltonians. However there is no contradiction in this fact, since the different Hamiltonians are expressed in terms of different variables. In the same sense, when we perform a canonical transformation we are free to select arbitrarily the generating function, [1] leading to different Hamiltonians expressed in terms of different canonical variables. For the same physical system, depending on the choice of the canonical variables, we can have completely different Hamiltonians, one being time-dependent and one being time-independent, or one being the energy of the system and one being not, and so on. [2]. All these different Hamiltonians describe the same physical system.

Let us consider now eq. (3.41) for $n = 1$ and let us choose the gauge function such that the equation

$$(m/2)\partial_\theta S_1 = -2\psi\epsilon U^0_{2m}\sin 2\theta, \tag{3.97}$$

[1] The choice of the gauge function is, however, subject to the restriction that it must be bounded in the variable φ.

[2] For a nice discussion see [5], sec. 8.2.

is satisfied. We then obtain

$$S_1 = U^0_{2m}\frac{2\psi\epsilon}{m}\cos 2\theta, \tag{3.98}$$

and, consequently, introducing the variable $\eta = \theta - (m/2)\varphi$, we obtain

$$\Gamma^1_\varphi = 2\epsilon' U^0_{20}\psi\sin 2\eta. \tag{3.99}$$

For the first order generators we obtain

$$g^\theta_1 = -U^0_{2m}\frac{2\epsilon}{m}\cos 2\theta, \tag{3.100}$$

$$g^\varphi_1 = -U^0_{2m}\frac{4\epsilon\psi}{m}\sin 2\theta + (2\psi)^{3/2}\frac{\cos\eta}{3}. \tag{3.101}$$

For the second order we need therefore to evaluate the quantity $C_2 = \gamma^2 - L_1\gamma^1 + (1/2)L^2_1\gamma^0$. After some lengthy algebra we arrive at the result [3]

$$\Gamma^2_\varphi = \epsilon'(2\psi)^{3/2}(1/6)U^0_{20}[-2\sin 2\eta\cos\eta - \cos 2\eta\sin\eta] + \frac{4\psi\epsilon^2}{m}U^{0\ 2}_{2m}. \tag{3.102}$$

Therefore, up to the second order, we have the following expression for the Hamiltonian

$$-H = \Gamma_\varphi = \Gamma^0_\varphi + \Gamma^1_\varphi + \Gamma^2_\varphi, \tag{3.103}$$

that is

$$\begin{aligned} H &= +(m/2)\psi - \epsilon' U^0_{20}2\psi\sin 2\eta \\ &\quad -\epsilon'(2\psi)^{3/2}(1/6)U^0_{20}[-2\sin 2\eta\cos\eta - \cos 2\eta\sin\eta] \\ &\quad -\frac{4\psi\epsilon^2}{m}U^{0\ 2}_{2m}. \end{aligned} \tag{3.104}$$

[3] We develop these calculations in ref. [14].

It can be seen that this Hamiltonian is time-independent, and therefore is integrable and cannot exhibit chaotic behavior. For another discussion on this problem, see ref. [15], pag. 130

3.7 Conclusion

We have derived in this chapter an expression for the Hamiltonian for the toroidal helical magnetic field lines system up to the second perturbative order for the cylindrical limit approximation of the field and up to the third perturbative order in the toroidal case. Going to higher orders will be a straightforward application of the same procedure used in this work, and the only difficulty to be expected is algebraic complication. The particular Hamiltonian we have derived is not the only possible choice, since we can manipulate the Lie transformation in order to get different Hamiltonians, and we have discussed this point in section 3.6, where a different Hamiltonian has been given up to the second order. Different expressions for the Hamiltonian could be of interest when analyzing particular problems, or for the application of symplectic integration schemes to the solution of Hamilton's equations.

Chapter 4

Symplectic Integration

4.1 Introduction

Hamiltonian systems possess in general many invariant, or conserved, quantities, which, depending on the particular system under consideration, may be the energy, the angular momentum and so on. Another invariant which is common to all Hamiltonian system is the phase space volume, which is a consequence of the conservation of differential form $\omega = dp^1 \wedge dq^1 + \cdots + dp^n \wedge dq^n$ and the exterior powers $\omega^2, \ldots, \omega^n$ by the flow of Hamiltonian systems. Notice that the conservation of ω prevents Hamiltonian systems from exhibiting dissipative dynamics.

Since only very seldom it is possible to find an analytical solution for the Hamilton equations, the use of numerical methods to integrate the equations of motion is common,

and it is natural to look for numerical methods that guarantee that, apart from round-off errors, the conserved quantities of a given Hamiltonian system are conserved also in the numerical integration process. Since the differential form ω is an invariant for all Hamiltonian systems, in the recent years much attention has been given to numerical schemes that conserve ω (see refs. [16], [17], [18], [19], [20], [21], [22]). These numerical schemes are usually called symplectic schemes, because the conservation of ω is equivalent to the request that the transformation $(q_n, p_n) \to (q_{n+1}, p_{n+1})$ between two successive time-steps is canonical (canonical transformations are also called symplectic transformations).

It should be noted here that for non integrable Hamiltonian systems it is not possible to have symplectic algorithms that conserve also the energy. In fact, if H is conserved by the numerical flow and if the original system has no other independent integrals, then for a symplectic algorithm the approximate and real flows are the same up to a reparametrization of time, and we would thus have solved the equations of motion (ref.[23]). [1]

However, even if the energy is not conserved by the symplectic method, there is no secular error in the energy, that is the error on the energy does not increase steadily with time, but is bounded, as a consequence of the fact that symplectic numerical schemes are by themselves Hamiltonian systems.

The symplectic integration of Hamiltonian systems is by now an established technique,

[1] This remark does not apply to linear Hamiltonian systems and to one-degree of freedom, time-independent Hamiltonians, which are integrable. For these systems it is therefore possible to have symplectic algorithms that conserve also the energy.

however many symplectic schemes are applicable only when the Hamiltonian is separable (that is of the form $H(p,q) = T(p) + V(q)$), or are not of very high order, and often a discussion of the numerical stability properties of the method lacks (a comparison of the accuracies of some symplectic integrators can be found in ref. [30]). While some merits of symplectic integration schemes are clearly demonstrated (refs. [16], [17], [20]) in a constant step-size environment, it is still not clear if it will be possible to keep the benefits of symplecticity in a variable step-size environment (ref. [22]). With this background in mind, we think that it is useful to look for new numerical methods applicable to Hamiltonian systems, as well as to ordinary differential equations.

In this chapter we will describe a new numerical scheme (ref. [24]) for the solution of initial value problems for ordinary differential equations. This work represents an attempt to modify, and possibly to improve, an algorithm developed by T. Watanabe et al. (refs. [25], [26]), called HIDMAS, with an eye towards applications in the field of Hamiltonian systems. The result of our efforts is a new numerical scheme of very high order and in possess of good stability properties. The principal difference with respect to HIDMAS is that while in HIDMAS all the grid points are chosen in a way similar to a collocation Runge-Kutta, in our scheme we have a number of fixed grid points and other grid points chosen in analogy to HIDMAS. This results in a higher order of accuracy with less computational effort. We will describe practically our algorithm until the order 14, and we will show that it is A-stable until the order 12. In section 4.5 we show how it is possible to put the scheme

in a Runge-Kutta form. Another characteristic of our scheme is that it is symplectic with respect to linear Hamiltonian systems. This is discussed in section 4.6. The coefficients that characterize our methods are given in the Appendix.

4.2 Symplectic Methods

Consider the Hamiltonian system

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}, \quad \frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}, \quad i = 1, 2, \ldots, N. \tag{4.1}$$

We know that when we transform the coordinates from $q = (q_1, q_2, ..., q_n)$, $p = (p_1, p_2, ..., p_n)$ to $Q = (Q_1, Q_2, ..., Q_N)$, $P = (P_1, P_2, ..., P_N)$, then the coordinate transformation is canonical if and only if the condition $M^t J M = J$ is satisfied. Here M is the Jacobian of the transformation and J is the matrix that has been defined in eq. (2.8). Also, we discussed in section 2.2 that, if $q = q(q_0, p_0, t)$, $p = p(q_0, p_0, t)$ is a solution of Hamilton's equations, then the coordinate transformation $(q_0, p_0) \to (q, p)$ is a canonical transformation, and therefore the symplectic condition $M^t J M = J$ is satisfied. In this case the Jacobian is given by

$$M = \begin{pmatrix} \frac{\partial}{\partial q_0} q & \frac{\partial}{\partial q_0} p \\ \frac{\partial}{\partial p_0} q & \frac{\partial}{\partial p_0} p \end{pmatrix}.$$

In numerical integration methods, the coordinates after an integration step are given by a mapping Ψ_h in phase space that effects the transition $(p_{n+1}, q_{n+1}) = \Psi_h(p_n, q_n)$. Thus the method is canonical if and only if the Jacobian of the above transformation is such that

the symplectic condition holds, that is it must be

$$\left(\frac{\partial \Psi_h}{\partial z}\right)^T J \left(\frac{\partial \Psi_h}{\partial z}\right) = J, \tag{4.2}$$

where we have introduced the notation $z = (q, p)$. When we are dealing with the numerical integration of Hamilton's equations, the use of non symplectic numerical methods may have a number of undesired consequences. Let us consider a simple example. For the one-dimensional harmonic oscillator with Hamiltonian $H = (1/2)(p^2 + q^2)$ we know the analytic solution and we also know that the energy is conserved. Suppose now that we want to integrate numerically the equation of motion for q and p and let us use the Euler method (non symplectic), which for a system of differential equations of the type

$$\frac{\partial}{\partial x} y = F(y), \tag{4.3}$$

makes use of the mapping

$$y\prime = y + hF(y). \tag{4.4}$$

Then, we find that an application of the Euler method to the harmonic oscillator problem gives, after one time step of length h

$$q\prime = q + hp, \qquad p\prime = p - hq, \tag{4.5}$$

and therefore we have

$$q\prime^2 + p\prime^2 = (1 + h^2)(q^2 + p^2). \tag{4.6}$$

We see that at each time step the value of the energy is multiplied by the factor $(1 + h^2)$, that is the system has been artificially excited by the numerical method. This kind of error, increasing steadily with time, is called a secular error. The use of a higher order, non symplectic method, like the classical fourth order Runge-Kutta, does not make things much better. It is in fact found in that case that (ref. [31])

$$q\prime^2 + p\prime^2 = (1 - (1/72)h^6 + \cdots)(q^2 + p^2), \tag{4.7}$$

so that we have an artificial damping of the system. The artificial damping is of much more small amplitude than the artificial excitation provoked by the Euler method is, but after many integration steps its effects will become evident anyway. For symplectic schemes in general the energy is not conserved, but there is no secular increase in the error. This is because a symplectic scheme is a Hamiltonian system itself, and therefore the numerical trajectory must lie on a surface of constant H_N, where H_N is the numerical Hamiltonian.

4.3 The Difference Scheme

To illustrate the difference scheme of our method, let us suppose that the equation to be integrated is of the form $y\prime(x) = F(x, y(x))$. Then, first the integration time step is subdivided into n subintervals of equal length by placing in the interval the points $0, h, 2h, ..., nh$. The number of unknowns is therefore $2(n+1)$, since we consider unknowns the quantities $y_0, y\prime_0, y_1, y\prime_1, ..., y\prime_n$. We have one initial condition (the value of y_0) and

$n+1$ equations $y'_0 = F(y_0), ..., y'_n = F(y_n)$, and therefore we need n more relations to close our scheme. To obtain the n relations we need to choose n points $s_1 h, ..., s_n h$, each for every sub-interval, and we write the equations $y'(s_1 h) = F(y(s_1 h)), ..., y'(s_n h) = F(y(s_n h))$. We now write the quantities $y(s_1 h), y'(s_1 h), ..., y'(s_n h)$ as

$$y(sh) = \sum_{j=0}^{n} \left[c_j(s) y(jh) + h d_j(s) y'(jh) \right], \tag{4.8}$$

$$y'(sh) = \sum_{j=0}^{n} \left[\frac{1}{h} g_j(s) y(jh) + f_j(s) y'(jh) \right]. \tag{4.9}$$

The coefficients obey the relations

$$c_j(n) = \delta_{jn}, \quad d_j(n) = 0, \quad g_j(n) = 0, \quad f_j(n) = \delta_{jn}.$$

We now determine the coefficients by expansion of the right hand side of the preceding equations about the point sh, and then by equating the coefficients of the derivatives of y. The Taylor expansion yields

$$y(sh) = \sum_{j=0}^{n} \sum_{l=0}^{\infty} \left[c_j(s) y^{(l)}(sh) h^l \frac{1}{l!} (j-s)^l + d_j(s) y^{(l+1)}(sh) h^{l+1} \frac{1}{l!} (j-s)^l \right], \tag{4.10}$$

$$y'(sh) = \sum_{j=0}^{n} \sum_{l=0}^{\infty} \left[g_j(s) y^{(l)}(sh) h^{l-1} \frac{1}{l!} (j-s)^l + f_j(s) y^{(l+1)}(sh) h^l \frac{1}{l!} (j-s)^l \right]. \tag{4.11}$$

The coefficients should be therefore determined by the relations

$$\delta_{l,0} = \sum_{j=0}^{n} \left[c_j(s) \frac{1}{l!} (j-s)^l + d_j(s) \frac{l}{l!} (j-s)^{l-1} \right], \tag{4.12}$$

$$\delta_{l,1} = \sum_{j=0}^{n} \left[g_j(s) \frac{1}{l!} (j-s)^l + f_j(s) \frac{l}{l!} (j-s)^{l-1} \right], \tag{4.13}$$

$$l = 0, .., 2n+1$$

where δ is the Kronecker symbol, since we need $2(2n+2)$ equations in order to determine all the coefficients in eqs. (4.10) and (4.11). This yields $y(sh)$ as an approximation of order $o(h^{2n+2})$ to the true solution and $y'(sh)$ as an approximation of order $o(h^{2n+1})$. To make the approximation of $y(sh)$ to be of the same order of the approximation of $y'(sh)$, we add one more equation for $y'(sh)$, precisely the equation obtained letting $l = 2n+2$ in eq. (4.13)

$$0 = \sum_{j=0}^{n} \left[g_j(s) \frac{1}{(2n+2)!} (j-s)^{2n+2} + f_j(s) \frac{1}{(2n+1)!} (j-s)^{2n+1} \right] \tag{4.14}$$

Since the coefficients $d_j(s)$ and $f_j(s)$ have already been determined (as functions of s) from eqs. (4.12) and (4.13), eq. (4.14) is an equation of degree $2n+1$ in the variable s. The $2n+1$ solutions are all real, and of these $n+1$ correspond to the points $s = 0, 1, ..., n$, since in these points eq. (4.14) is automatically satisfied. The remaining n solutions correspond to points which lie in the n sub-intervals, as can be seen from Fig. 4.1. These n solutions give us n sets of coefficients, which characterize the method for the given order n.

4.3.1 Implementation

Once the coefficients have been obtained, we have to solve simultaneously the following system of equations

$$Y_i = \sum_{k=0}^{n} \left[c_{ik} y_k + h d_{ik} F(x_k, y_k) \right], \tag{4.15}$$

$$F(s_i h, Y_i) = \sum_{k=0}^{n} \left[\frac{1}{h} g_{ik} y_k + f_{ik} F(x_k, y_k) \right], \tag{4.16}$$

with $i = 1, ..., n$, and the notation $y(s_i h) = Y_i$ is used. That is, after substitution of eq. (4.15) into eq. (4.16), we have to solve simultaneously a system of n equations from which we get the n values $y_1, ..., y_n$. As discussed in section 4.3 the order of the solution is $o(h^{2n+2})$, and this is true for every value $y_1, ..., y_n$, in contrast with Runge-Kutta methods like the Gauss-Legendre method or the Lobatto methods, for which the intermediate values are of lower order with respect to the final value y_n. A more detailed comparison between these methods and our method is presented in section 4.4.

4.3.2 Truncation Error

The expressions for the truncation errors of $y, y\prime$ are

$$\Delta y(sh) = \delta y(sh) h^{2n+2} y(sh)^{(2n+2)} + o(h^{2n+2}),$$

$$\Delta y\prime(sh) = \delta y\prime(sh) h^{2n+2} y(sh)^{(2n+3)} + o(h^{2n+2}),$$

where

$$\delta y(sh) = \sum_{j=0}^{n} \left[c_j(s) \frac{1}{(2n+2)!} (j-s)^{2n+2} + d_j(s) \frac{1}{(2n+1)!} (j-s)^{2n+1} \right],$$

$$\delta y\prime(sh) = \sum_{j=0}^{n} \left[g_j(s) \frac{1}{(2n+3)!} (j-s)^{2n+3} + f_j(s) \frac{1}{(2n+2)!} (j-s)^{2n+2} \right],$$

are problem independent coefficients. Plots for n=1,2,3,4,5,6 of $\delta y(sh)$ and $\delta y\prime(sh)$ are shown in Fig. 4.2 and Fig. 4.3.

4.4 Accuracy and Stability of the Method

To test the accuracy and the stability of the method we have applied it to the solution of the test equation

$$y\prime(x) = -\lambda y(x), \quad y(0) = 1, \quad \lambda \in \mathcal{C}, \tag{4.17}$$

for the cases $n = 1, 2, 3, 4, 5, 6$. Though eq. (4.17) is very simple, its use as a model to predict the stability behavior of numerical methods for general nonlinear systems is very widespread. The exact solution of (4.17) is $y(x) = \exp(-Re(\lambda x))$, and its module is given by $\mid y(x) \mid = \exp(-Re(\lambda x))$. The module of the exact solution is not increasing if $Re(\lambda x) \geq 0$, therefore it is natural to require that a numerical method, when applied to (4.17), gives

$$\mid y_{n+1} \mid \leq \mid y_n \mid, \tag{4.18}$$

if $Re(\lambda h) \geq 0$. By definition the region of absolute stability of the method is the region for which $\mid y \mid < 1$. If this region comprises the half-plane $Re(h\lambda) > 0$, then the method is said to be A-stable (see ref. [32], pag. 374-378).

We give below the expression for $y\prime(x)$ in the case $n = 5$. The length of the step in this case is $5h$. The solution $y\prime(x)$ can be written as

$$y(5h) = \frac{A(\lambda)}{A(-\lambda)},$$

where

$$\begin{aligned} A(\lambda) \;=\; & 9979200 - 24948000\, h\,\lambda + 29862000\, h^2\,\lambda^2 - 22680000\, h^3\,\lambda^3 \\ & +12199320\, h^4\,\lambda^4 - 4904550\, h^5\,\lambda^5 + 1512075\, h^6\,\lambda^6 \\ & -359250\, h^7\,\lambda^7 + 64538\, h^8\,\lambda^8 - 8220\, h^9\,\lambda^9 + 600\, h^{10}\,\lambda^{10}. \end{aligned}$$

The Taylor expansion of $y(5h) - \exp(-5h\lambda)$ yields

$$y(5h) - \exp(-5h\lambda) \;= \frac{-144425}{230150688768}\lambda^{13}h^{13} + o(h)^{14},$$

which differs from the expansion of $\exp(-5h\lambda)$ to the order $o(h^{13})$. The accuracy is of the same order also for the intermediate values of y. The discretization for $n = 5$ is of order $o(h^{12})$, but in this case when we solve for y the accuracy is raised by one. So, with respect to the test equation, for a given n our method is accurate up to $o(h^{2n+3})$, and we say that the method has order $2n + 2$. Since for a given n we have to solve n simultaneous equations, as explained in section 4.3.1, we can compare our method with Runge-Kutta schemes which require the simultaneous solution of the same number of equations. Restricting

ourselves to the Gauss-Legendre and the Lobatto methods, it is known (ref. [33]) that the n-stages Gauss-Legendre and the $(n + 1)$-stages Lobatto methods both require the simultaneous solution of n equations and have order of accuracy $2n$. Therefore, for the same computational effort, our method provides a higher order than the aforementioned methods. Besides, for our method the order is the same also for all the intermediate values, in contrast to the Gauss-Legendre and Lobatto methods for which the order drops in the intermediate stages.

We note that when λ is pure imaginary, then $\mid \frac{A(\lambda)}{A(-\lambda)} \mid = 1$. This is reflected also in Fig. 4.4, where we plotted the contours of y as a function of the complex argument λh corresponding to the values $\mid y \mid = 0.5, 1, 1.5$. In the figure the line corresponding to $\mid y \mid = 1$ is the straight line which corresponds to a pure imaginary λh. It can be seen that the method is A-stable for $n = 1, 2, 3, 4, 5$, while the A-stability property is lost for $n = 6$. This is a consequence of the fact that the zeros of the denominator of the solution cross the axis $Re(h\lambda) = 0$ for $n = 6$ (see Fig. 4.5). Investigation about the A-stability property for $n > 6$ has not been done, but Fig. 4.5 suggests that the A-stability property may be lost for $n > 6$. This contrasts with Gauss-Legendre and Lobatto methods, which are A-stable for every order (ref. [33]).

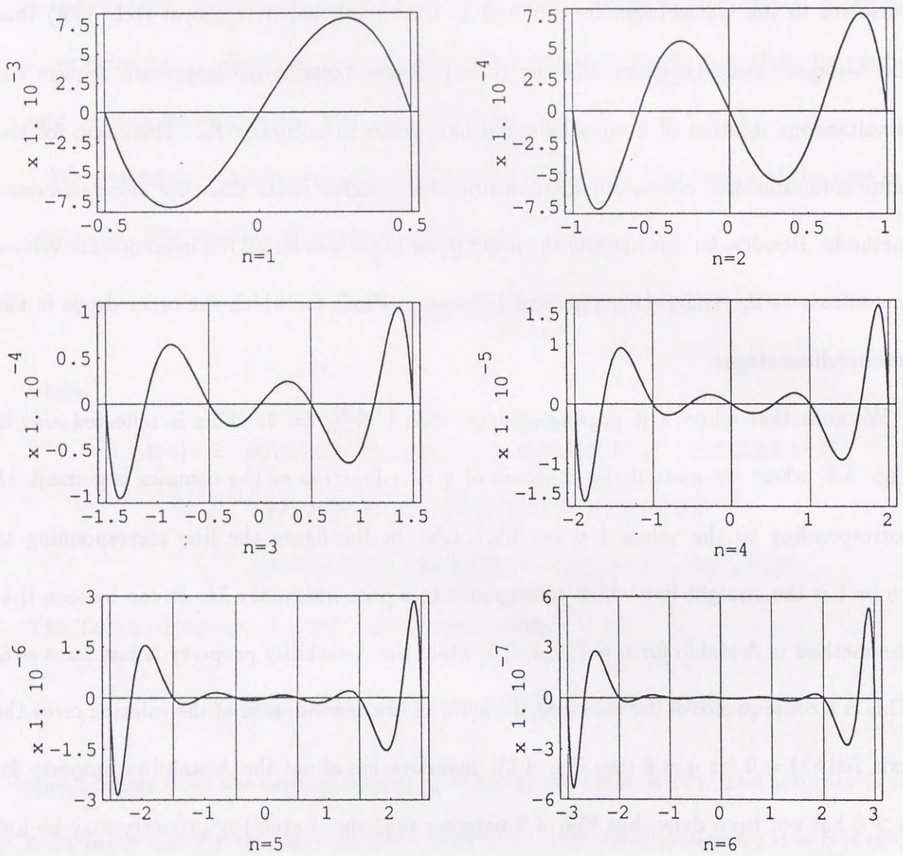

Figure 4.1: Plots of the r.h.s. of eq. 4.14 for $n = 1, \ldots, 6$.

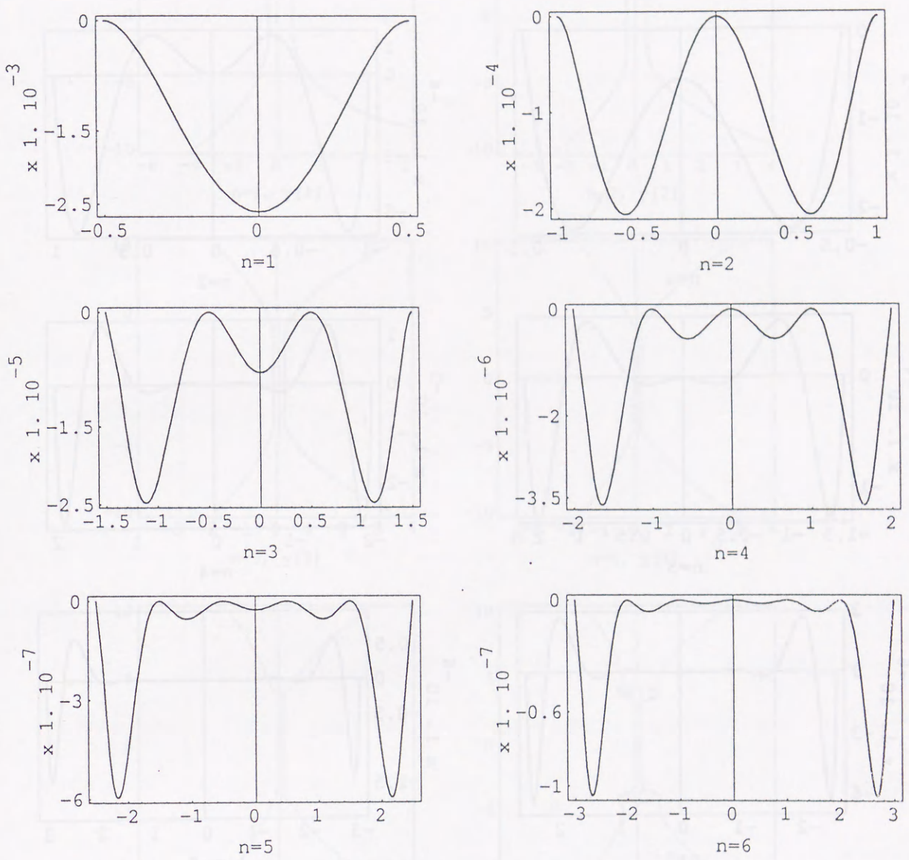

Figure 4.2: Plots of the truncation error for y.

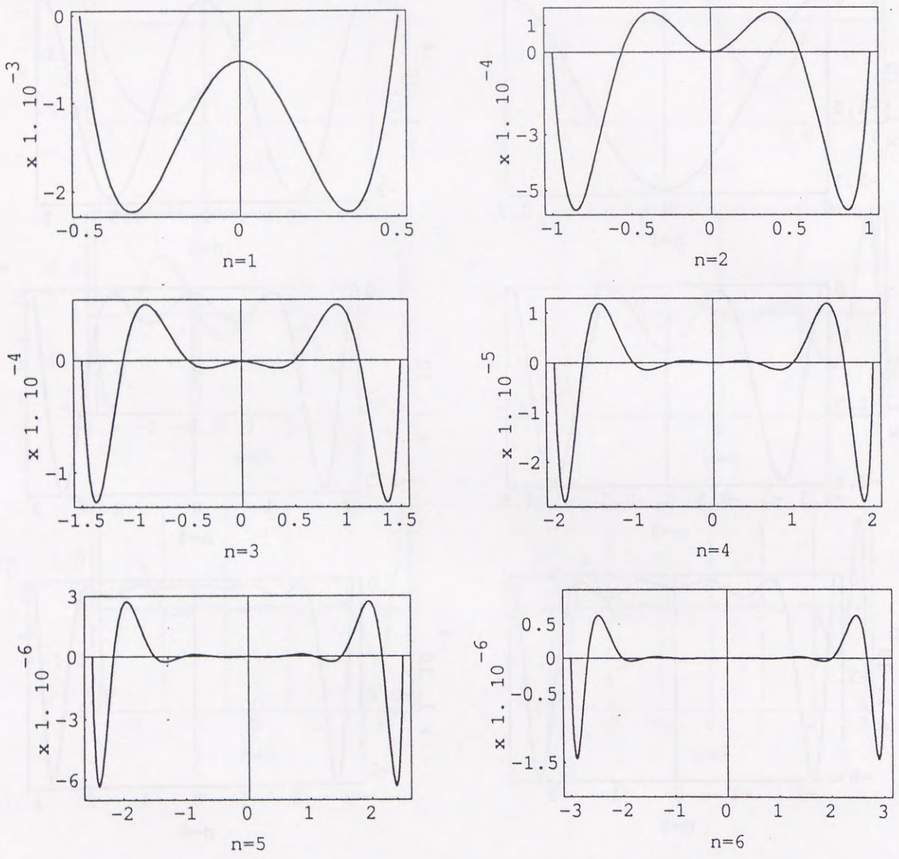

Figure 4.3: Plots of the truncation error for $y\prime$.

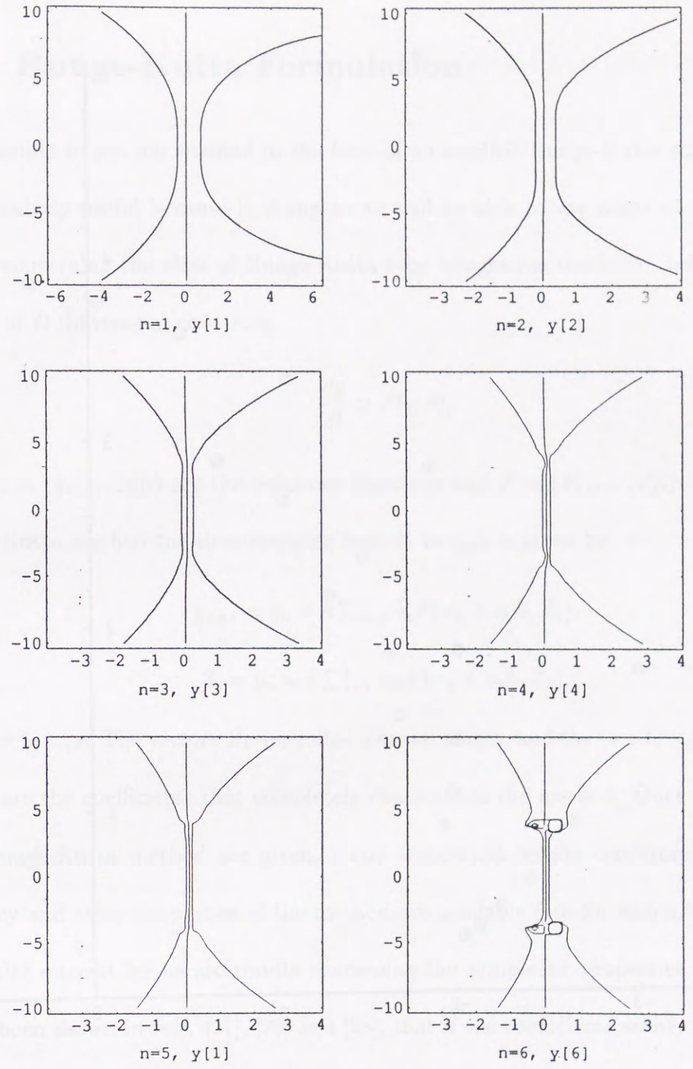

Figure 4.4: Plots of the contours of $\mid y \mid$. On the left of each figure the contour corresponding to $\mid y \mid = 1.5$, in the center $\mid y \mid = 1$, on the right $\mid y \mid = 0.5$. Horizontal axis: $Re(\lambda h)$. Vertical axis: $Im(\lambda h)$.

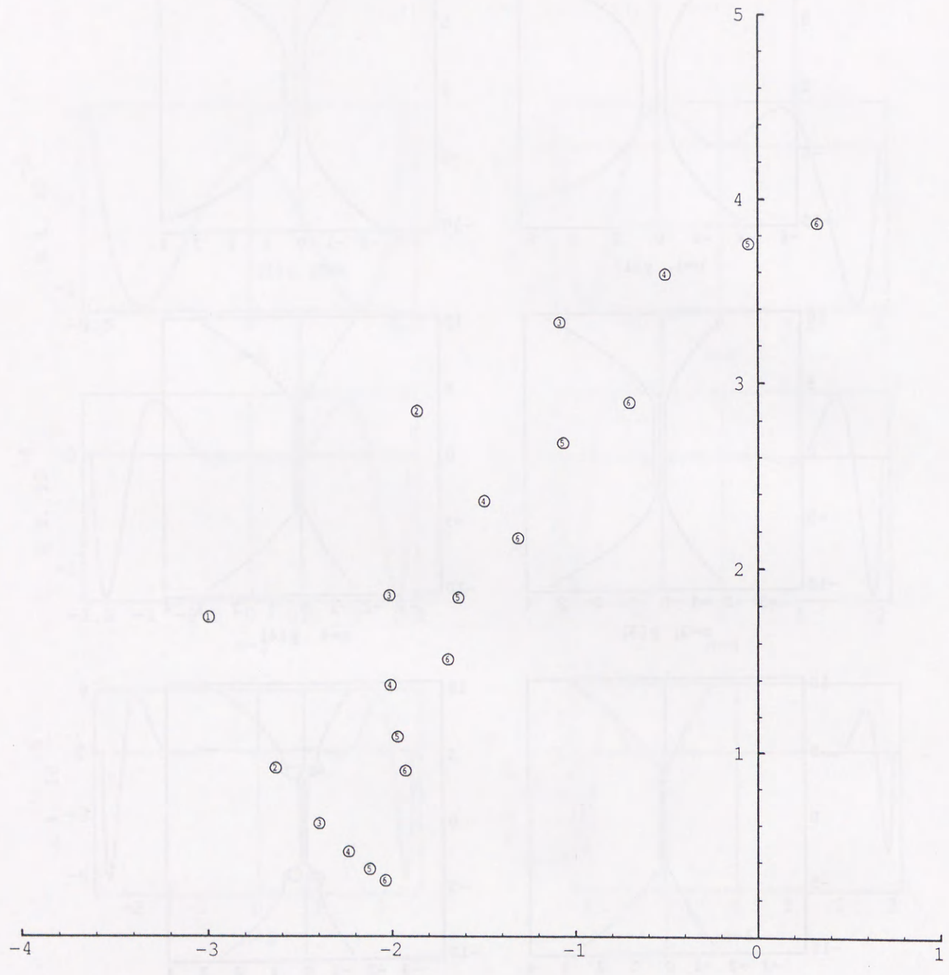

Figure 4.5: Distribution of the zeros of the denominator of $A(\lambda)/A(-\lambda)$, solution of the test equation $y' = -\lambda y$, for n=1,...,6. Inside the circles the corresponding n is indicated. The vertical axis is $Re(\lambda h)$, the horizontal axis is $Im(\lambda h)$. The zeros are symmetrical with respect to the horizontal axis.

4.5 Runge-Kutta Formulation

It is possible to put our method in the form of an implicit Runge-Kutta scheme, and this is particularly useful because in doing so we will be able to use many of the theoretical results concerning the class of Runge-Kutta type integration methods. Let us consider a system of D differential equations

$$\frac{dy}{dt} = F(y,t), \tag{4.19}$$

where $y = (y_1, \ldots, y_D)$ are the unknown functions and $F = (F_1, \ldots, F_D)$. For an s-stage Runge-Kutta method the time-stepping from t_n to t_{n+1} is given by

$$\begin{aligned} y_{n+1} &= y_n + h\sum_{k=1}^{s} b_k F(x_n + c_k h, Z_k), \\ Z_i &= y_n + h\sum_{k=1}^{s} a_{ik} F(x_n + c_k h, Z_k), \end{aligned} \tag{4.20}$$

with $i = 1, ..., s$. The vectors Z_k are called internal stages, and the $(s+1) \times s$ real constants b_k, a_{ik} are the coefficients that completely characterize the method. Once the coefficients of a Runge-Kutta method are given, many theoretical results concerning the stability, accuracy and other properties of the method are available (see for example ref. [33]). Of particular interest for us are results concerning the symplectic properties of the method. It has been shown in refs. [27], [29] and [28], that if the coefficients satisfy the relation

$$m_{ij} = b_i a_{ij} + b_j a_{ji} - b_i b_j = 0, \quad i,j = 1, \ldots, s, \tag{4.21}$$

then the method is symplectic.

Let us now show how our method can be put in a Runge-Kutta form. We start by writing eqs. (4.15) and (4.16) in the form

$$Y_i = c_{i0}y_0 + c_{ik}y_k + hd_{i\mu}\dot{y_\mu} \tag{4.22}$$

$$\dot{Y_i} = \frac{1}{h}g_{i0}y_0 + \frac{1}{h}g_{ik}y_k + f_{i\mu}\dot{y_\mu} \tag{4.23}$$

with the convention that we have to sum from 1 to n if two indexes are equal. The summation is from 1 to n if the indexes are Latin and from 0 to n if the indexes are Greeks. Now, if the matrix g_{ik} is invertible, multiplying eq. (4.23) by g_{ji}^{-1} we obtain

$$g_{ji}^{-1}\dot{Y_i} = \frac{1}{h}g_{ji}^{-1}g_{i0}y_0 + \frac{1}{h}\delta_{jk}y_k + g_{ji}^{-1}f_{i\mu}\dot{y_\mu},$$

that is

$$y_j = -g_{ji}^{-1}g_{i0}y_0 + hg_{ji}^{-1}(\dot{Y_i} - f_{i\mu}\dot{y_\mu}).$$

Substituting in eq. (4.22), we obtain

$$\begin{aligned} Y_i &= c_{i0}y_0 - c_{ik}g_{kl}^{-1}g_{l0}y_0 + hc_{ik}g_{kl}^{-1}(\dot{Y_l} - f_{l\mu}\dot{y_\mu}) \\ &\quad + hd_{i\mu}\dot{y_\mu}. \end{aligned}$$

Now, if in eqs. (4.15) and (4.16) we consider the function $y = 1$, we can derive the relations $g_{ji}^{-1}g_{i0} = -1$, $c_{i0} - c_{ik}g_{kl}^{-1}g_{l0} = 1$, $j = 1, ..., n$, so that we obtain

$$y_j = y_0 + h(g_{jl}^{-1}(\dot{Y_l} - f_{l\mu}\dot{y_\mu})),$$

$$Y_i = y_0 + h(c_{ik}g_{kl}^{-1}(\dot{Y_l} - f_{l\mu}\dot{y_\mu}) + d_{i\mu}\dot{y_\mu}).$$

Now, remembering that $\dot{Y_l} = F(x_0 + s_l h, Y_l)$, $\dot{y_\mu} = F(x_0 + \mu h, y_\mu)$ and defining the quantities $V_0 = y_0$, $V_i = y_i$, $i = 1, ..., n$, we obtain

$$V_j = y_0 + h(g_{jl}^{-1}(F(x_0 + s_l h, Y_l) - f_{l\mu}F(x_0 + \mu h, V_\mu))),$$

$$Y_i = y_0 + h(c_{ik}g_{kl}^{-1}(F(x_0 + s_l h, Y_l) + (d_{i\mu} - c_{ik}g_{kl}^{-1}f_{l\mu})F(x_0 + \mu h, V_\mu)).$$

We obtain therefore the following Runge-Kutta scheme

$$y_n = y_0 + h(g_{nl}^{-1}(F(x_0 + s_l h, Y_l) - f_{l\mu}F(x_0 + \mu h, V_\mu))),$$

$$Y_i = y_0 + h(c_{ik}g_{kl}^{-1}(F(x_0 + s_l h, Y_l) + (d_{i\mu} - c_{ik}g_{kl}^{-1}f_{l\mu})F(x_0 + \mu h, V_\mu)),$$

$$V_j = y_0 + h(g_{jl}^{-1}(F(x_0 + s_l h, Y_l) - f_{l\mu}F(x_0 + \mu h, V_\mu))),$$

$$V_0 = y_0.$$

Comparing with (4.20) we see that our scheme can also be considered as a $2n + 1$ stages Runge-Kutta process, with a step-length nh, and coefficients given by

$$nb_\mu = -g_{nk}^{-1}f_{k\mu}, \quad na_{i\mu} = -g_{ik}f_{k\mu}, \quad na_{i+n,\mu} = d_{i\mu} - c_{ik}g_{kl}^{-1}f_{l\mu},$$

$$nb_{i+n} = g_{ni}^{-1}, \qquad na_{i,j+n} = g_{ij}^{-1}, \qquad na_{i+n,j+n} = c_{ik}g_{kj}^{-1},$$

with $i, j = 1, ..., n$, $\mu = 0, ..., n$ and $a_{0i} = 0$ for $i = 0, ..., 2n$. For n=1 and n=2 the coefficients are given below. In the last row of the matrices are the coefficients b_i. It is

interesting to note that for $n = 1$, a permutation of the rows and columns shows that our method is equivalent to a Runge-Kutta of the Lobatto III-A type with 3 stages.

$$\begin{pmatrix} 0 & 0 & 0 \\ 1/6 & 1/6 & 2/3 \\ 5/24 & -1/24 & 1/3 \\ 1/6 & 1/6 & 2/3 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ \frac{31}{480} & \frac{2}{15} & \frac{1}{480} & \frac{3\left(8+5\sqrt{3}\right)}{160} & \frac{3\left(8-5\sqrt{3}\right)}{160} \\ \frac{1}{15} & \frac{4}{15} & \frac{1}{15} & \frac{3}{10} & \frac{3}{10} \\ \frac{81+2\sqrt{3}}{1080} & \frac{2\left(9-7\sqrt{3}\right)}{135} & \frac{-9+2\sqrt{3}}{1080} & \frac{18+\sqrt{3}}{120} & \frac{3\left(2-\sqrt{3}\right)}{40} \\ \frac{81-2\sqrt{3}}{1080} & \frac{2\left(9+7\sqrt{3}\right)}{135} & \frac{-\left(9+2\sqrt{3}\right)}{1080} & \frac{3\left(2+\sqrt{3}\right)}{40} & \frac{18-\sqrt{3}}{120} \\ \frac{1}{15} & \frac{4}{15} & \frac{1}{15} & \frac{3}{10} & \frac{3}{10} \end{pmatrix}$$

Now, if we apply the condition 4.21, we see that our method cannot be proven to be symplectic. In fact, for $n = 1$ we obtain

$$m_{ij} = \begin{pmatrix} -1/36 & 0 & 1/36 \\ 0 & 1/36 & -1/36 \\ 1/36 & -1/36 & 0 \end{pmatrix}.$$

4.6 Linear Symplectic Methods

In this section we show that our method is indeed a linear symplectic method. By linear symplectic methods we intend integration methods which are symplectic only for the class of Hamiltonians of the form $H = z^T R z$, where $z = (q_1, \ldots, q_n, p_1, \ldots, p_n)$ and R is a $2n \times 2n$ square matrix. In the case of two degrees of freedom this expression reduces to $H = \alpha p^2 + \beta q^2 + \gamma qp$. The one-dimensional harmonic oscillator is a member of this class. Let us now proceed to study the linear symplectic properties of our method. The system of equations that we have to solve is

$$Y_i = \sum_{k=0}^{n} \left[c_{ik} y_k + h d_{ik} F(x_k, y_k) \right], \tag{4.24}$$

$$\dot{Y}_i = \sum_{k=0}^{n} \left[\frac{1}{h} g_{ik} y_k + f_{ik} F(x_k, y_k) \right], \tag{4.25}$$

and, when applied to the Hamilton equations, we obtain

$$\tilde{q}_i = \sum_{k=0}^{n} \left[c_{ik} q_k + h d_{ik} G(q_k, p_k) \right], \tag{4.26}$$

$$\tilde{\dot{q}}_i = \sum_{k=0}^{n} \left[\frac{1}{h} g_{ik} q_k + f_{ik} G(q_k, p_k) \right], \tag{4.27}$$

$$\tilde{p}_i = \sum_{k=0}^{n} \left[c_{ik} p_k + h d_{ik} F(q_k, p_k) \right], \tag{4.28}$$

$$\tilde{\dot{p}}_i = \sum_{k=0}^{n} \left[\frac{1}{h} g_{ik} p_k + f_{ik} F(q_k, p_k) \right], \tag{4.29}$$

where we have used the notation $\dot{p} = F(q,p)$, $\dot{q} = G(q,p)$ and $\tilde{q}_i$, $\tilde{\dot{q}}_i$, $\tilde{p}_i$, $\tilde{\dot{p}}_i$ correspond to $\dot{Y}_i$, Y_i. Differentiating we obtain

$$d\tilde{q}_i = \sum_{k=0}^{n} \left[c_{ik} dq_k + h d_{ik} \left(\frac{\partial G}{\partial q_k} dq_k + \frac{\partial G}{\partial p_k} dp_k \right) \right], \tag{4.30}$$

$$d\tilde{\dot{q}}_i = \sum_{k=0}^{n} \left[\frac{1}{h} g_{ik} dq_k + f_{ik} \left(\frac{\partial G}{\partial q_k} dq_k + \frac{\partial G}{\partial p_k} dp_k \right) \right], \tag{4.31}$$

$$d\tilde{p}_i = \sum_{k=0}^{n} \left[c_{ik} dp_k + h d_{ik} \left(\frac{\partial F}{\partial q_k} dq_k + \frac{\partial F}{\partial p_k} dp_k \right) \right], \tag{4.32}$$

$$d\tilde{\dot{q}}_i = \sum_{k=0}^{n} \left[\frac{1}{h} g_{ik} dp_k + f_{ik} \left(\frac{\partial F}{\partial q_k} dq_k + \frac{\partial F}{\partial p_k} dp_k \right) \right]. \tag{4.33}$$

Now, we have

$$d\tilde{\dot{q}}_i = \frac{\partial G}{\partial \tilde{q}_i} d\tilde{q}_i + \frac{\partial G}{\partial \tilde{p}_i} d\tilde{p}_i, \tag{4.34}$$

$$d\tilde{\dot{p}}_i = \frac{\partial F}{\partial \tilde{q}_i} d\tilde{q}_i + \frac{\partial F}{\partial \tilde{p}_i} d\tilde{p}_i, \tag{4.35}$$

and therefore, substituting these relations into (4.30) $\sim$ (4.33), and then substituting (4.30) into (4.31) and (4.32) into (4.33) we obtain a linear system of $2n$ equations in the $2n+2$ unknowns $dq_0, dq_1, \ldots, dq_n, dp_0, dp_1, \ldots, dp_n$, which we solve for $dq_1, \ldots, dq_n, dp_1, \ldots, dp_n$,

obtaining

$$dq_i = a^i_{11} dq_0 + a^i_{12} dp_0, \tag{4.36}$$

$$dp_i = a^i_{21} dq_0 + a^i_{22} dp_0, \tag{4.37}$$

for $i = 1, \ldots, n$. Now, for a symplectic method we must have that the relation $dq_n \wedge dp_n = dq_0 \wedge dp_0$ is satisfied, that is it must be

$$a^n_{11} a^n_{22} - a^n_{12} a^n_{21} = 1. \tag{4.38}$$

The coefficients $a^n_{11}, a^n_{22}, a^n_{12}, a^n_{21}$ depend on the coefficients $c_{ik}, d_{ik}, g_{ik}, f_{ik}$, and on the derivatives $\frac{\partial F}{\partial q_k}, \frac{\partial F}{\partial p_k}, \frac{\partial F}{\partial \tilde{q}_k}, \frac{\partial F}{\partial \tilde{p}_k}, \frac{\partial G}{\partial q_k}, \frac{\partial G}{\partial p_k}, \frac{\partial G}{\partial \tilde{q}_k}, \frac{\partial G}{\partial \tilde{p}_k}$ and the relation (4.38) is not satisfied for our method. However, for a linear Hamiltonian all these derivatives are constants, and using a computer algebra program we have verified that (4.38) is satisfied for $n = 1, 2, 3$ and 4. We can therefore conclude that the integration scheme is linearly symplectic for these values of n, and we conjecture that it is a linear symplectic scheme also for higher values of n.

4.7 Conclusion

We have presented in this chapter a new numerical scheme of very high order, suitable for the solution of initial values problems for ordinary differential equations. The method is A-stable until the order twelve, and this, together with considerations about the distribution of

the truncation error, suggests that maybe the orders between eight and twelve are the best choice for many problems. The method has also proven to be symplectic with respect to linear Hamiltonians, a characteristic that could be useful even when nonlinear Hamiltonian systems are integrated. Numerical experiments on the symplectic properties of the method and its application to a magnetic field flow problem will be presented in the next chapter. In the Appendix the coefficients until the order fourteen are explicitly and exactly given.

Chapter 5

Numerical Results

5.1 Introduction

In this chapter we apply our method to the solution of the Hamilton equations obtained for the magnetic field lines system. The numerical results described in this chapter are obtained using the coefficients corresponding to $n = 4$, which give a method of order 10. These coefficients are given explicitly in the Appendix. The method is then implemented in a program written in RATFOR (ref. [34]) . The step length h is held fixed, $h = 2.45 \times 10^{-2}$ and for every time-step the program proceeds using the Newton-Raphson method to solve the system of equations given by (4.15) and (4.16). For a Hamiltonian system of n degrees of freedom this implies that the Newton-Raphson routine must solve a system of $4 \times 2n$ equations at every time-step. We tested the algorithm on the two-

body Kepler motion problem, on the vibrating beams Hamiltonian (ref. [16]) and on the two-resonances Hamiltonian $H = p^2/2 + 2\pi\epsilon(\cos(2\pi q) + \cos(2\pi(q - t)))$. In the case of the Kepler problem no secular error on the energy and the angular momentum has been observed. In the case of the vibrating beams Hamiltonian no secular error on the energy has appeared.

5.2 Toroidal Hamiltonian

In this section we present the numerical results concerning the third order Hamiltonian derived in section 3.5. At the first and second order the Hamiltonian does not reproduce in a satisfactory manner the chaotic behavior of the toroidal helical magnetic field, so we describe here the third order results. The Hamiltonian contains two smallness parameters, ϵ and ϵ', connected respectively to the inverse aspect ratio and to the intensity of the vertical field, which we can vary in each calculation. For a given choice of ϵ and ϵ', we present the Poincaré section taken at $\varphi = 0$, that is we plot the intersection points of the magnetic field lines with the plane XZ. The equations for the magnetic field lines are obtained applying Hamilton's equations

$$\dot{\theta} = \frac{\partial}{\partial\varphi}H, \qquad \dot{\psi} = -\frac{\partial}{\partial\varphi}H,$$

to the third order Hamiltonian derived in section 3.5. The points are plotted at intervals in φ of length $(2\pi)/5$ because of the periodicity of the Hamiltonian. This results in 5 times

less computer time for the same amounts of plot points.

For small values of ϵ and ϵ' the Poincaré section does not show any sign of chaotic behavior. Typically there is formation of magnetic islands as the radial distance ψ increases, but when ψ reaches a certain critical value the orbits tend to escape abruptly instead of giving the characteristic random distribution of the chaotic domain. This can be seen in Fig. 5.1. The straight line on the right represents the chosen initial conditions. At a certain critical initial condition the magnetic line does not wind around the torus forming a magnetic surface, but escapes abruptly and is not even seen in the plot, except for a few scattered points. In Fig. 5.2 we can observe the same behavior. We plot here starting from groups of seven close initial conditions, that is for each initial value of ψ we choose 7 close values of θ, so that each line in Fig. 5.2 corresponds in reality to 7 different lines. As ϵ or ϵ' or both are increased, this behavior gradually changes and the formation of a stochastic layer begins to take place (Figs. 5.3, 5.4 and 5.5). For $\epsilon = 0.023$ and $\epsilon' = 0.1$ the chaotic region appears clearly. In Fig. 5.6 a detail of the Poincaré section is shown. The five straight lines on the top right are the initial conditions. Also in this case we have orbits confined on magnetic surfaces and orbits that escape out of the plot when ψ is big enough, but in between there are orbits that intersect the XZ plane in many random points before eventually escape. In Fig. 5.7 we plot only three orbits. While one orbit originates an island structure, the other two wander around quite randomly. In Figs. 5.8 and 5.9 two examples of the rotational transform ι are presented. The horizontal axis corresponds to

ψ. The quite scattered points after $\psi \sim 0.1$ are due to the fact that the magnetic field line escapes after a few revolutions. The power law decrease of ι agrees quite nicely with the theoretical prediction of ref. [35]. We can conclude that the third order Hamiltonian derived in section 3.5 reproduces reasonably well the behavior of the field lines system and that it can be used as a basis for more detailed numerical investigations.

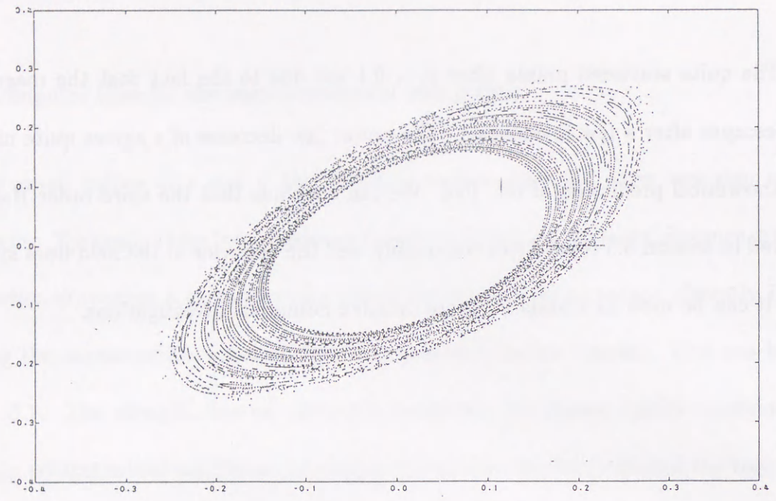

Figure 5.1: Poincare' section for $\epsilon = 0.023$, $\epsilon' = 0.02$. The straight line on the right represents the initial conditions.

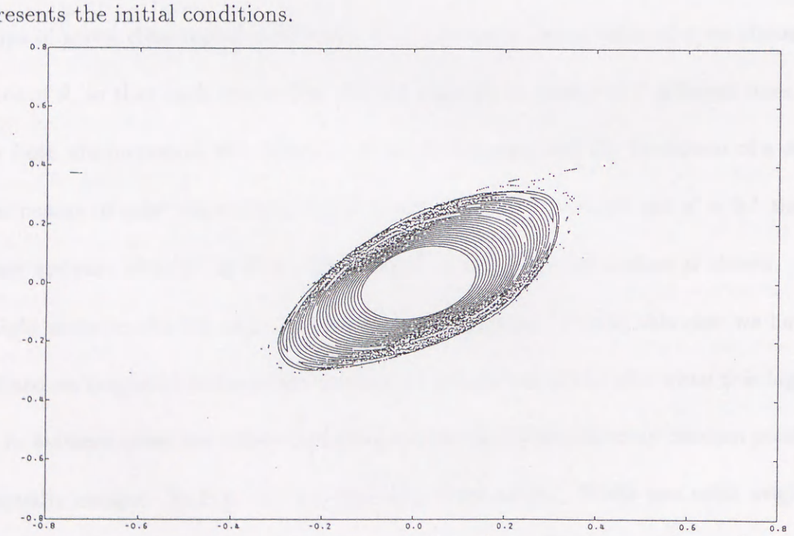

Figure 5.2: Poincare' section for $\epsilon = 0.02$, $\epsilon' = 0.02$, for groups of 7 close initial conditions.

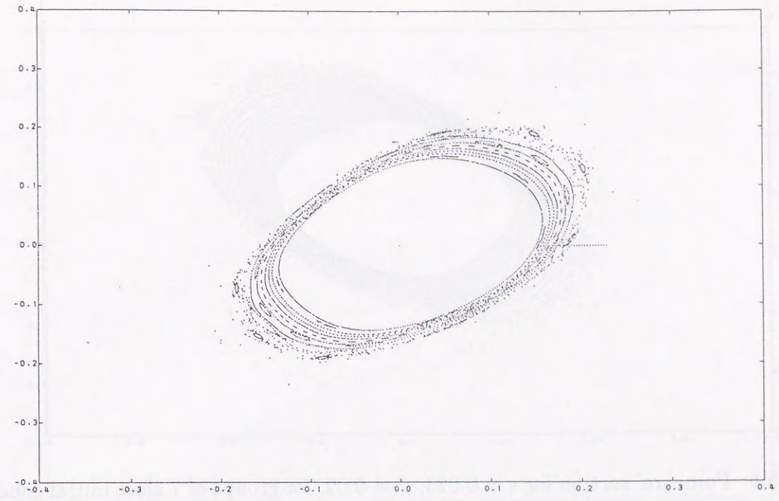

Figure 5.3: Poincare' section for $\epsilon = 0.0245$, $\epsilon' = 0.09$. The straight line on the right represents the initial conditions.

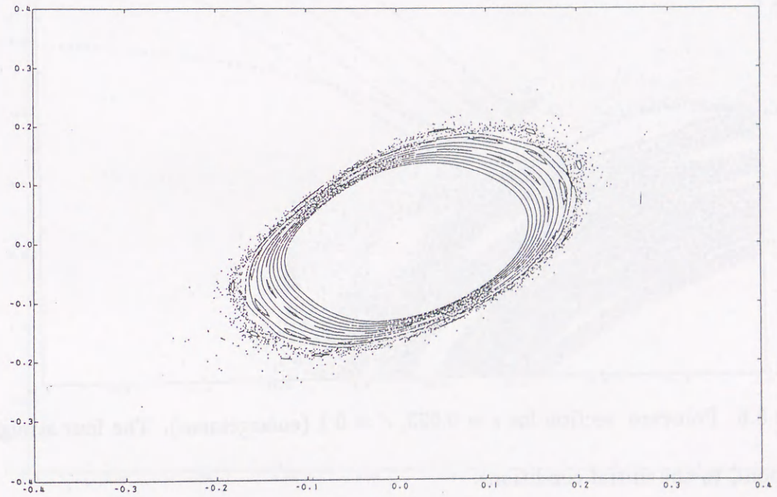

Figure 5.4: Poincare' section for $\epsilon = 0.0245$, $\epsilon' = 0.09$, for groups of 7 close initial conditions.

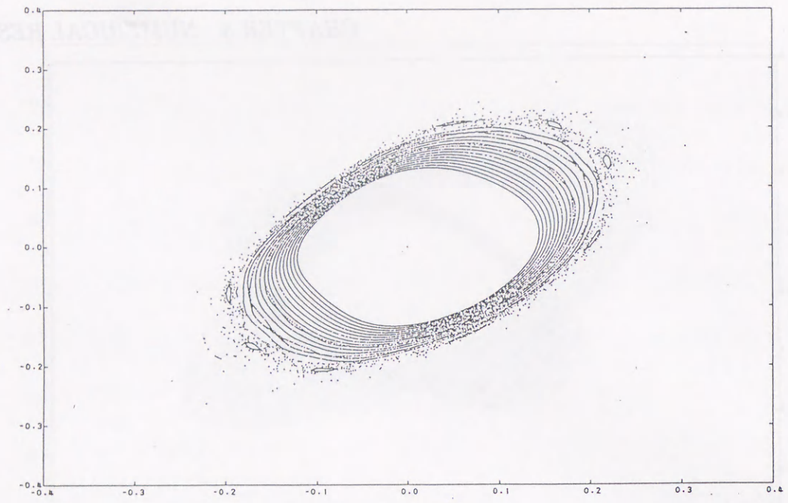

Figure 5.5: Poincare' section for $\epsilon = 0.023$, $\epsilon' = 0.09$, for groups of 7 close initial conditions.

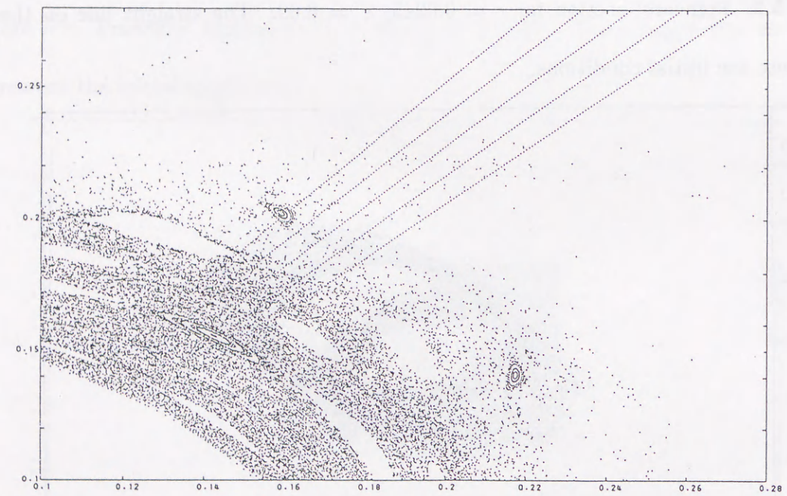

Figure 5.6: Poincare' section for $\epsilon = 0.023$, $\epsilon' = 0.1$ (enlargement). The four straight lines correspond to the initial conditions.

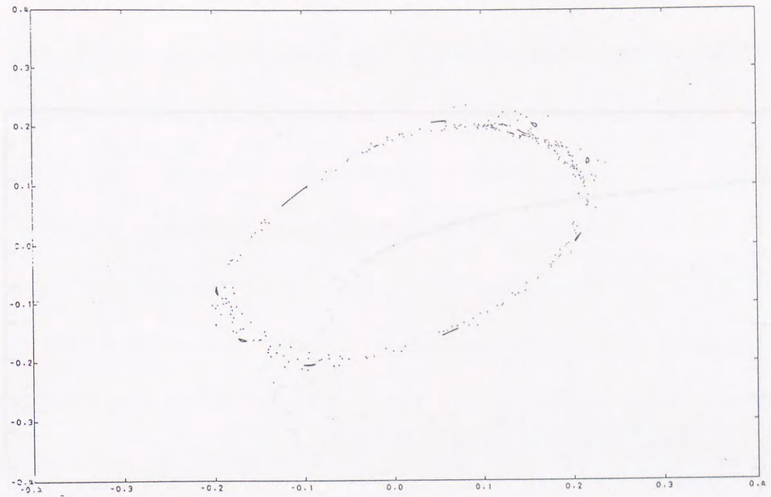

Figure 5.7: Plot of three initial conditions, $\epsilon = 0.023$, $\epsilon' = 0.1$.

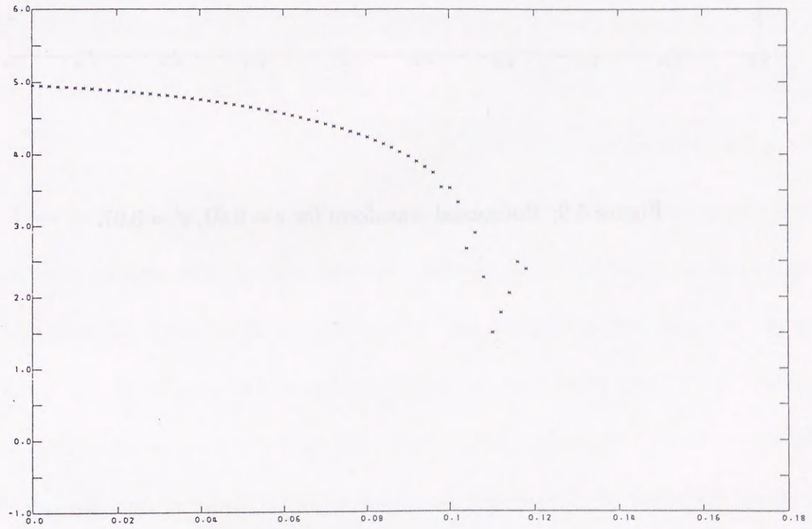

Figure 5.8: Rotational transform for $\epsilon = 0.03$, $\epsilon' = 0.04$.

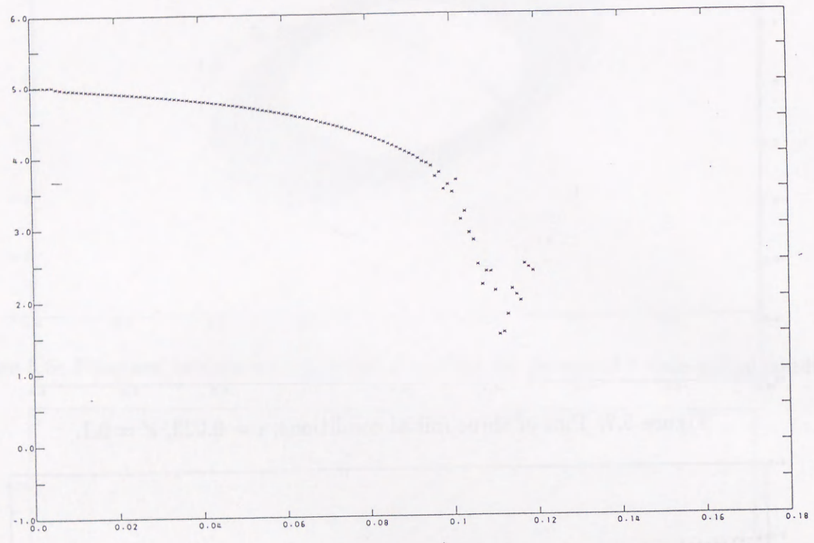

Figure 5.9: Rotational transform for $\epsilon = 0.03$, $\epsilon' = 0.07$.

Chapter 6

Concluding Remarks

The two main results of this thesis are the derivation of a Hamiltonian for the helical magnetic field in the vacuum and the construction of a new linear symplectic scheme suitable for its numerical integration.

We have derived the Hamiltonian applying a perturbation theory based on the Lie transform, a systematic procedure to calculate the expansion to high orders. After obtaining a Hamiltonian for the cylindrical limit approximation of the field, we have derived the Hamiltonian for the general toroidal case up to the third order. We have also derived an integrable model for the same toroidal case. The existence of these two different Hamiltonians for the same physical system is related with the choice of the variables when we apply the Lie perturbation technique, and probably also with the asymptotic character of the expansion itself. Research on the relation between these two models is being currently

done, and we plan to study the convergence properties of the expansion scheme in the near future. Also, a renormalization approach which makes use of a more realistic form for the unperturbed Hamiltonian and gives a better convergence, is being currently investigated.

We have then presented the construction of a linear symplectic integration scheme. The scheme is of very high order, and has also good stability properties. We have shown that it is A-stable until the order twelve. Contrarily to many existing symplectic methods, our method is applicable to every Hamiltonian system [1] and not only to special classes of Hamiltonian systems. The choice to use a linear symplectic scheme for the integration of a nonlinear system is ultimately judged by numerical experiments. Numerical tests on known models have been carried out and have confirmed its good performances. Its application to the magnetic field lines problem has shown that the Hamiltonian we have derived is able to reproduce the regular and chaotic behavior of the field.

[1] The scheme is also applicable to differential equations in general.

Appendix A

Coefficients

A.1 Introduction

In this appendix we give the explicit form of the coefficients of the integration scheme for $n = 1, ..., 6$. While in the case $n = 1$ it is still possible to calculate the coefficients by hands, as n increase the algebra is still elementary but quite lengthy and it becomes useful, if not necessary, to use a computer algebra program to perform automatically the analytical calculations. We have used the program MATHEMATICA. In what follows, the case $n = 1$ is treated in detail, with the purpose of illustration, while for the remaining cases we give only the results.

A.2 The case n=1

For n = 1 we obtain an integration scheme of the fourth order. Eqs. (4.12) and (4.13) now read

$$\delta_{l,0} = \sum_{j=0}^{1}[c_j(s)\frac{1}{l!}(j-s)^l + d_j(s)\frac{1}{(l-1)!}(j-s)^{l-1}], \tag{A.1}$$

$$\delta_{l,1} = \sum_{j=0}^{1}[g_j(s)\frac{1}{l!}(j-s)^l + f_j(s)\frac{1}{(l-1)!}(j-s)^{l-1}], \tag{A.2}$$

where $l = 0, 1, 2, 3$. Solving these equations, for the new variable $p = s + 1/2$, we obtain the coefficients

$$\begin{aligned}
&c_0(p) = 1/2 - (3/2)p + 2p^3, && c_1(p) = 1/2 + (3/2)p - 2p^3 = c_0(-p),\\
&d_0(p) = 1/8 - p/4 - p^2/2 + p^3, && d_1(p) = -1/8 - p/4 + p^2/2 + p^3 = -d_0(-p),\\
&g_0(p) = -3/2 + 6p^2, && g_1(p) = 3/2 - 6p^2 = -g_0(-p),\\
&f_0(p) = -1/4 - p + 3p^2, && f_1(p) = -1/4 + p + 3p^2 = f_0(-p).
\end{aligned} \tag{A.3}$$

Substituting the coefficients into eq. (4.14) we obtain the equation

$$p^3 - p/4 = 0, \tag{A.4}$$

which has solutions $p = -1/2, 0, 1/2$. The solution $p = 0$ gives us therefore the set of coefficients

$$\begin{aligned}
&c_0 = \tfrac{1}{2}, \quad c_1 = \tfrac{1}{2}, \quad d_0 = \tfrac{1}{8}, \quad d_1 = -\tfrac{1}{8},\\
&g_0 = -\tfrac{3}{2}, \quad g_1 = \tfrac{3}{2}, \quad f_0 = -\tfrac{1}{4}, \quad f_1 = -\tfrac{1}{4},
\end{aligned} \tag{A.5}$$

which will be used to solve the differential equation.

A.3 The cases n = 2, 3, 4, 5, 6

The results are obtained following the same procedure described for the case n = 1. We give below $D(p)$, which is defined to be the right hand side of eq. (4.14), and the solutions of $D(p) = 0$ which lie in the sub-intervals, and the coefficients for n = 2, 3, 4, 5. The variable p is defined as $p = s - n/2$.

A.3.1 n = 2

$$D(p) = \frac{(1-p)\ p\ (1+p)\ (-1+3\,p^2)}{360}, \tag{A.6}$$

$$p_1 = -\frac{1}{\sqrt{3}}, \quad p_2 = -p_1.$$

The coefficients are given below. Attention should be paid to the fact that the expressions below are valid only for the particular values p_1, p_2, and not for every p in the interval $-1, 1$. This is a consequence of the fact that the full expressions of the coefficients are in general quite long and we have chosen to use a simplified expression valid only for the solutions p_1, p_2. This is not a loss of generality, because the coefficients which characterize the method are the ones corresponding to the solutions p_1, p_2. So, the first set of coefficients is obtained substituting in the expressions below p_1 for p, and the second substituting p_2 for p. The same kind of remark applies also to the cases n = 3, 4, 5, 6, with the obvious difference that the number of roots increases.

$$\begin{aligned}
&c_0(p) = \tfrac{5-6\,p}{18}, \qquad c_2(p) = c_0(-p),\\
&c_1(p) = \tfrac{4}{9},\\
&d_0(p) = \tfrac{1-p}{18}, \qquad d_2(p) = -d_0(-p),\\
&d_1(p) = \tfrac{4\,p}{9},\\
&g_0(p) = \tfrac{-5+8\,p}{6}, \qquad g_2(p) = -g_0(-p),\\
&g_1(p) = \tfrac{-8\,p}{3},\\
&f_0(p) = -\tfrac{1}{9} + \tfrac{p}{6}, \quad f_2(p) = f_0(-p),\\
&f_1(p) = -\tfrac{4}{9}.
\end{aligned} \tag{A.7}$$

A.3.2 n = 3

$$D(p) = \frac{p\ (-3+2\,p)\ (-1+2\,p)\ (1+2\,p)\ (3+2\,p)\ (5-4\,p^2)}{322560}, \tag{A.8}$$

$$p_1 = \frac{-\sqrt{5}}{2}, \quad p_2 = 0, \quad p_3 = -p_1.$$

For the solution p_2 we have

$$\begin{aligned}
&c_0(p_2) = \tfrac{1}{4}, \quad c_1(p_2) = \tfrac{1}{4}, \quad c_2(p_2) = \tfrac{1}{4}, \quad c_3(p_2) = \tfrac{1}{4},\\
&d_0(p_2) = \tfrac{1}{24}, \quad d_1(p_2) = -\tfrac{1}{8}, \quad d_2(p_2) = \tfrac{1}{8}, \quad d_3(p_2) = -\tfrac{1}{24},\\
&g_0(p_2) = -\tfrac{185}{216}, \quad g_1(p_2) = \tfrac{5}{8}, \quad g_2(p_2) = -\tfrac{5}{8}, \quad g_3(p_2) = \tfrac{185}{216},\\
&f_0(p_2) = -\tfrac{7}{72}, \quad f_1(p_2) = -\tfrac{3}{8}, \quad f_2(p_2) = -\tfrac{3}{8}, \quad f_3(p_2) = -\tfrac{7}{72}.
\end{aligned} \tag{A.9}$$

For the solutions p_1, p_3 we have

$$\begin{aligned}
c_0(p) &= \tfrac{1}{4} - \tfrac{5p}{27}, & c_3(p) &= c_0(-p),\\
c_1(p) &= \tfrac{1}{4}, & c_2(p) &= c_1(-p),\\
d_0(p) &= \tfrac{1}{24} - \tfrac{p}{36}, & d_3(p) &= -d_0(-p),\\
d_1(p) &= -\tfrac{1}{8} + \tfrac{p}{4}, & d_2(p) &= -d_1(-p),\\
g_0(p) &= \tfrac{-185+162p}{216}, & g_3(p) &= -g_0(-p),\\
g_1(p) &= \tfrac{5-6p}{8}, & g_2(p) &= -g_1(-p),\\
f_0(p) &= \tfrac{-7+6p}{72}, & f_3(p) &= f_0(-p),\\
f_1(p) &= \tfrac{-3+2p}{8}, & f_2(p) &= f_1(-p).
\end{aligned} \tag{A.10}$$

A.3.3 n = 4

$$D(p) = \frac{(-2+p)(-1+p)p(1+p)(2+p)(-4+15p^2-5p^4)}{1814400}, \tag{A.11}$$

$$\begin{aligned}
p_1 &= -\tfrac{\sqrt{15+\sqrt{145}}}{\sqrt{10}}, & p_2 &= -\tfrac{\sqrt{15-\sqrt{145}}}{\sqrt{10}},\\
p_3 &= -p_2, & p_4 &= -p_1.
\end{aligned} \tag{A.12}$$

The numerical values are

$$p_1 = -1.64443\cdots, \quad p_2 = -0.543912\cdots.$$

The coefficients are

$$\begin{aligned}
c_0(p) &= \tfrac{-416+220p+2060p^2-1105p^3}{21600}, & c_4(p) &= c_0(-p),\\
c_1(p) &= \tfrac{404-560p-95p^2+260p^3}{1350}, & c_3(p) &= c_1(-p),\\
c_2(p) &= \tfrac{44-5p^2}{100},\\
d_0(p) &= \tfrac{-8+4p+50p^2-25p^3}{3600}, & d_4(p) &= -d_0(-p),\\
d_1(p) &= \tfrac{52-52p-55p^2+55p^3}{450}, & d_3(p) &= -d_1(-p),\\
d_2(p) &= \tfrac{p\left(44-5p^2\right)}{100},\\
g_0(p) &= \tfrac{444-256p-1587p^2+952p^3}{4320}, & g_4(p) &= -g_0(-p),\\
g_1(p) &= \tfrac{-276+448p+159p^2-208p^3}{270}, & g_3(p) &= -g_1(p),\\
g_2(p) &= \tfrac{p\left(-32+11p^2\right)}{10},\\
f_0(p) &= \tfrac{36-20p-135p^2+80p^3}{3600}, & f_4(p) &= f_1(-p),\\
f_1(p) &= \tfrac{-48+100p-60p^2+5p^3}{450}, & f_3(p) &= f_1(-p),\\
f_2(p) &= \tfrac{-44+5p^2}{100}.
\end{aligned} \tag{A.13}$$

A.3.4 n = 5

$$D(p) = p\,(-5+2p)\,(-3+2p)\,(-1+2p)\,(1+2p)\,(3+2p)\,(5+2p)\,\times$$
$$(-259+280\,p^2-48\,p^4)/(122624409600),$$

$$p_1 = \frac{-\sqrt{35+8\sqrt{7}}}{2\sqrt{3}}, \quad p_2 = \frac{-\sqrt{35-8\sqrt{7}}}{2\sqrt{3}}, \tag{A.14}$$
$$p_3 = 0, \qquad p_4 = -p_2, \qquad p_5 = -p_1.$$

The numerical values are

$$p_1 = -2.16345\cdots, \quad p_2 = -1.0737\cdots.$$

The coefficients are, for the solution p_3

$$\begin{aligned}
&c_0(p_3) = \tfrac{447}{262144}, && c_1(p_3) = \tfrac{10625}{262144}, && c_2(p_3) = \tfrac{1875}{4096},\\
&c_3(p_3) = \tfrac{1875}{4096}, && c_4(p_3) = \tfrac{10625}{262144}, && c_5(p_3) = \tfrac{447}{262144},\\
&d_0(p_3) = \tfrac{45}{131072}, && d_1(p_3) = \tfrac{1875}{131072}, && d_2(p_3) = \tfrac{5625}{32768},\\
&d_3(p_3) = -\tfrac{5625}{32768}, && d_4(p_3) = -\tfrac{1875}{131072}, && d_5(p_3) = -\tfrac{45}{131072},\\
&g_0(p_3) = -\tfrac{483}{655360}, && g_1(p_3) = -\tfrac{4375}{131072}, && g_2(p_3) = -\tfrac{13125}{8192},\\
&g_3(p_3) = \tfrac{13125}{8192}, && g_4(p_3) = \tfrac{4375}{131072}, && c_q(p_3) = \tfrac{483}{655360},\\
&f_0(p_3) = -\tfrac{9}{65536}, && f_1(p_3) = -\tfrac{625}{65536}, && f_2(p_3) = -\tfrac{5625}{16384},\\
&f_3(p_3) = -\tfrac{5625}{16384}, && f_4(p_3) = -\tfrac{625}{65536}, && f_5(p_3) = -\tfrac{9}{65536}.
\end{aligned} \tag{A.15}$$

For the solutions p_1, p_2, p_4, p_5 we have

$$\begin{aligned}
&c_0(p) = \tfrac{-306125+128870p+282500p^2-119096p^3}{4374000}, && c_5(p) = c_0(-p),\\
&c_1(p) = \tfrac{12825-11354p-3348p^2+3848p^3}{34992}, && c_4(p) = c_1(-p),\\
&c_2(p) = \tfrac{445-392p+68p^2+176p^3}{2187}, && c_3(p) = c_2(-p),\\
&d_0(p) = \tfrac{-2675+1070p+2540p^2-1016p^3}{291600}, && d_5(p) = -d_0(-p),\\
&d_1(p) = \tfrac{2103-1402p-1212p^2+808p^3}{11664}, && d_4(p) = -d_1(-p),\\
&d_2(p) = \tfrac{-83+166p-52p^2+104p^3}{1458} && d_3(p) = -d_2(-p)\\
&g_0(p) = \tfrac{2602985-1188750p-2280308p^2+1047000p^3}{8748000}, && g_5(p) = -g_0(-p),\\
&g_1(p) = \tfrac{-88235+76950p+25244p^2-20088p^3}{69984}, && g_4(p) = -g_1(-p),\\
&g_2(p) = \tfrac{8015-8430p-1724p^2+1464p^3}{8748}, && g_3(p) = -g_2(-p),\\
&f_0(p) = \tfrac{16385-7410p-14468p^2+6600p^3}{583200}, && f_5(p) = f_0(-p),\\
&f_1(p) = \tfrac{563+1494p-3020p^2+936p^3}{23328}, && f_4(p) = f_1(-p),\\
&f_2(p) = \tfrac{2(-88+93p-20p^2-12p^3)}{729}, && f_3(p) = f_2(-p).
\end{aligned} \tag{A.16}$$

A.3.5 n = 6

$$D(p) = (-3+p)\,(-2+p)\,(-1+p)\,p\,(1+p)\,(2+p)\,(3+p)\,\times$$
$$(36 - 147\,p^2 + 70\,p^4 - 7\,p^6)/(43589145600),$$

$$p_1 = -2.67804\cdots, \quad p_2 = -1.59578\cdots, \quad p_3 = -0.530655\cdots,$$
$$p_4 = -p_3, \qquad p_5 = -p_2, \qquad p_6 = -p_1.$$

The coefficients are

$$c_0(p) = \tfrac{27780-9660\,p-98987\,p^2+34349\,p^3+36743\,p^4-12761\,p^5}{5292000}, \quad c_6(p) = c_0(-p),$$
$$c_1(p) = \tfrac{-415+245\,p+2366\,p^2-1393\,p^3-399\,p^4+252\,p^5}{12250}, \qquad c_5(p) = c_1(-p),$$
$$c_2(p) = \tfrac{452-644\,p-91\,p^2+259\,p^3+7\,p^4-7\,p^5}{1568}, \qquad c_4(p) = c_2(-p),$$
$$c_3(p) = \tfrac{4\left(159-77\,p^2+14\,p^4\right)}{1323},$$
$$d_0(p) = \tfrac{180-60\,p-609\,p^2+203\,p^3+231\,p^4-77\,p^5}{264600}, \qquad d_6(p) = -d_0(-p),$$
$$d_1(p) = \tfrac{3\left(-10+5\,p+56\,p^2-28\,p^3-14\,p^4+7\,p^5\right)}{2450}, \qquad d_5(p) = -d_1(-p),$$
$$d_2(p) = \tfrac{3\left(8-8\,p-7\,p^2+7\,p^3\right)}{196}, \qquad d_4(p) = -d_2(-p),$$
$$d_3(p) = \tfrac{4\,p\left(159-77\,p^2+14\,p^4\right)}{1323},$$

(A.17)

$$g_0(p) = \tfrac{-96588+36036\,p+377661\,p^2-139831\,p^3-134661\,p^4+50023\,p^5}{4536000}, \quad g_6(p) = -g_0(-p),$$
$$g_1(p) = \tfrac{547-316\,p-2184\,p^2+1336\,p^3+309\,p^4-188\,p^5}{3500}, \qquad g_5(p) = -g_1(-p),$$
$$g_2(p) = \tfrac{-508+812\,p+465\,p^2-557\,p^3-57\,p^4+61\,p^5}{448}, \qquad g_4(p) = -g_2(-p),$$
$$g_3(p) = \tfrac{2\,p\left(-981+506\,p^2-53\,p^4\right)}{567},$$
$$f_0(p) = \tfrac{-2028+756\,p+7861\,p^2-2891\,p^3-2821\,p^4+1043\,p^5}{1058400}, \qquad f_6(p) = f_0(-p),$$
$$f_1(p) = \tfrac{12-21\,p-84\,p^2+126\,p^3-56\,p^4+7\,p^5}{4900}, \qquad f_5(p) = f_1(-p),$$
$$f_2(p) = \tfrac{-228+420\,p-105\,p^2-63\,p^3-7\,p^4+7\,p^5}{1568}, \qquad f_4(p) = f_2(-p),$$
$$f_3(p) = \tfrac{4\left(-159+77\,p^2-14\,p^4\right)}{1323}.$$

(A.18)

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