Optimized stellarator magnetic fields

Master Thesis
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Abstract

One of the main shortcomings of stellarators is their neoclassical transport. Indeed, the presence of unconfined particle orbits can lead to prohibitively high transport levels. In order to guarantee confinement properties comparable to tokamaks, it was first proposed that stellarators be quasisymmetric, meaning that they exhibit a symmetry direction analogous to axial symmetry in tokamaks. The good neoclassical properties displayed by quasisymmetric configurations were further generalized to omnigeneous configurations, i.e. a less restrictive condition for which, in like manner, all particles experience vanishing average radial drifts. Although this augmentation in the degrees of freedom brings about its amount of theoretical and practical complexities, it might lead to the finding of e.g. low-aspect-ratio stellarators displaying good transport confinement which was proved to be impracticable in the context of quasisymmetric configurations. As transport optimization of existing stellarators consists in bringing their magnetic configurations closer to omnigeneity, it is important to derive and test both analytical and numerical tools that permit to describe omnigeneous configurations.

With this aim, in 1997, Cary and Sasharina obtained a mathematical expression that, given the second adiabatic invariant and the value of the magnetic field strength on (roughly) half a flux-surface, yields the value of the latter on the rest of it. This general equation is, among other things, a useful tool for investigating omnigeneous magnetic configurations.

As a primary task, this work recapitulates the theoretical background on neoclassical transport necessary to grasp the entire study and provide the reader with an accurate intuition of the physics behind the equations. Furthermore, the derivation of the above-mentioned mathematical expression is revisited, numerically implemented and tested through simulations on both a quasisymmetric configuration and an omnigeneous configuration that is far from being quasisymmetric. The former is an idealization of the configuration of the Helically Symmetric eXperiment (HSX), and the latter relies on methods to construct omnigeneous magnetic fields proposed by Landreman in 2012 (which are based on Cary and Sasharina’s work).

Keywords: Stellarator, optimization, omnigeneity, second adiabatic invariant.
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Chapter 1

Introduction

Global demand for energy is increasing at a daunting rate by dint of population growth and expanding access to electricity worldwide. As the capacity of the earth system to absorb greenhouse gas emissions is already exhausted, the Paris agreement on climate stands that emissions must cease by 2040 or 2050. This requires to swap fossil fuels against a sustainable, carbon-free form of energy that can operate at large-scale. The deuterium-tritium (D-T) fusion reaction

\[ \text{D} + \text{T} \rightarrow \text{He} + \text{n} + 17.6 \text{ MeV}, \]

stands as a candidate thanks to its inherent advantages. 1) Fusion does not emit greenhouse gases into the atmosphere, neither does it produce high activity, long-lived nuclear waste. Its major by-product is helium that is an inert, non-toxic gas. 2) There is no risk of meltdown as, in any case of disturbance, the plasma cools down and the reaction stops. 3) Fusion reactants are virtually inexhaustible and globally available. Indeed, tritium will be produced during the fusion reaction while deuterium can be processed directly from water which is not only favourable to sustainability but also to the world economy.

A lot of effort has been put into harnessing fusion from the mid-nineties on. The most promising approach is thermonuclear fusion, which endows fusion reactions by rising the reactants temperature up to the order of 100 million degrees. In order to sustain the reactions, the fuel, that is at the state of plasma for such high temperatures, must be contained. The main approach to achieve plasma containment bears the name of Magnetic Confinement Fusion (MCF). It consists in using torus-shaped magnetic fields with nested magnetic flux surfaces as a trap for the particles (cf. figure 1.1). Magnetic flux surfaces are mathematically defined as

\[ \vec{B}(\vec{r}) \cdot \vec{n}(\vec{r}) = 0, \quad \forall \vec{r} \in S, \]

where \( \vec{B} \) is the magnetic field, \( \vec{r} \) the position vector, \( \vec{n} \) the surface’s normal and \( S \) is the fluxed surface.

The idea behind MCF is that, at fusion-relevant temperature, all particles are charged and charged particles follow the magnetic field lines by orbiting around them. However because of the complex shape of such MCF machines, the magnetic field lines must be twisted. There are two main ways to do so: generating the desired magnetic field through complex twisted magnetic coil systems or inducing a toroidal electric current so that, by Ampère’s law, the particles contribute to providing the magnetic field in which they are trapped. Stellarators embody the first approach while tokamaks make use of the second one.
Almost seven decades have passed now since the invention of the stellarator concept by Lyman Spitzer in 1951. At that time, the race for providing energy to the fast-developing world through the implementation of a nuclear fusion facility was at its start. Despite coming ahead in time, stellarators have grown in the shadow of their axi-symmetric cousin, the tokamak. This is probably mostly due to historical reasons and the engineering complexity of building relevant magnetic coil systems for stellarators. Indeed, as tokamaks require toroidal current that is inductively generated, they display a pulsed behavior whereas stellarator do not require toroidal current and therefore are intrinsically better fitted for steady state operation. Another critical issue engendered by the toroidal current in tokamaks resides in the presence of plasma-terminating disruptions caused by current driven instabilities. Those unstable modes (i.e. kink modes, sawteeth, resistive and neo-classical tearing modes) all limit the plasma performance and are driven by the tendency of two conducting wires, that is, in the context of MCF, flux tubes, with parallel currents to repel each other. Current instabilities are almost non-existent in stellarators as there is no substantial toroidal current. As a benchmark, after 120,000 plasma discharges, LHD has still not experienced a single current driven disruption [2]. What is more, in stellarators, the plasma density is not limited by the Greenswald limit [3], and this quantity has a huge impact on the feasibility of a fusion reactor as not only does the fusion triple product $n\tau_E T$, which roughly determines the output power, depend directly on density but the confinement time does too.

The numerous benefits of stellarators, however, come not only at the price of complicated manufacturing. In 1967 already, it was observed that there are always some particle orbits that are unconfined, regardless of the magnetic field strength [4]. This can lead to deleterious neoclassical transport (i.e. the transport of particles due to Coulomb collisions).

In order to achieve good transport levels, it was first proposed that stellarators be quasisymmetric [5]. Before defining quasisymmetry, let us first clarify a few notions:

- A set of flux coordinates is one that includes a flux surface label defined as a single-valued function that is constant on each flux surface. Put in another way, calling $\psi$ the flux coordinate, to each $\psi$ corresponds a single flux surface.

- Magnetic coordinates are a particular type of flux coordinates associated with...
straight magnetic field lines, i.e. for a fixed value of \( \psi \), the magnetic field lines are traced by a linear combination of the other coordinates.

- In the presence of e.g. a radial electric field \( \vec{E} \), the ions in the plasma experience a drift in the \( \vec{E} \times \vec{B}/B^2 \) direction. For \( \vec{E} = -\nabla \phi \sim \nabla \psi \), with \( \phi \) the electrostatic potential, this flow goes in the \( \nabla \psi \times \vec{B} \) direction, called the diagmagnetic direction. The Boozer coordinates \((\psi, \theta, \zeta)\) are magnetic coordinates for which the diamagnetic lines are straight. This system of coordinates is represented in figure 1.1.

A quasisymmetric magnetic configuration is one for which the magnetic-field strength depends on a single linear combination of the toroidal flux angles i.e.

\[
B(\psi, \theta, \zeta) \equiv B(\psi, m\theta - n\zeta),
\]  

(1.1)

where \( \psi, \theta \) and \( \zeta \) are Boozer coordinates, and \( m \) and \( n \) are integers.

Quasisymmetric stellarators have shown confinement times at least as good as the ones associated with tokamaks of similar size [6]. Furthermore, quasisymmetric magnetic fields transport theory is closely related to that of axisymmetric systems.

Later, the good neoclassical properties displayed by quasi-symmetric configurations were further generalized to omnigeneous configurations, that is configurations for which secular radial drifts vanish. This mathematically translates into

\[
\frac{1}{\tau_b} \int_{\text{orb.}} \frac{dl}{v_\parallel} \vec{v}_d \cdot \nabla \psi = 0,
\]  

(1.2)

where \( \tau_b \) is the period of the parallel motion, i.e. time for a particle to trace an orbit. \( \vec{v}_d \) is the drift velocity, \( v_\parallel \) is the component of the velocity parallel to the magnetic field lines and the integral is performed over an orbit trajectory. Introducing the notation \( \langle ... \rangle_{\text{orb.}} \) for the orbit-average, equation (1.2) reads

\[
\langle \vec{v}_d \cdot \nabla \psi \rangle_{\text{orb.}} = 0.
\]  

(1.3)

One of the advantages of the generalization to omnigeneous configurations is the possibility of prototyping low-aspect-ratio stellarators with good transport properties while it has been shown to be impossible for quasisymmetric stellarators [7].

Let \( l \) denote the arc length traveled along a field line. In their pioneering work on the study of neoclassical transport optimization for stellarators, Cary and Sasharina developed a formula that, given the second adiabatic invariant

\[
J = \oint_{\text{orb.}} dl \left| v_\parallel(l) \right|
\]  

(1.4)

and the value of the magnetic field strength on (roughly) half a flux-surface, yields the value of the latter on the rest of it.

In this work, the theoretical resources associated with the field of neoclassical optimization in stellarators are firstly put forward. In particular it is shown that trapped particles follow trajectory that conserve the second adiabatic invariant \( J \). The expression found by Cary and Sasharina is then derived and studied. Eventually, its numerical implementation is discussed and the results provided thereby are described.
1. Introduction
Chapter 2

Theoretical background

2.1 Compendium on magnetic coordinates

The magnetic configuration can be quite intricate in magnetic confinement fusion (MCF) machines. This tends to make any computation difficult. Changing the system of coordinates may allow one to sweep the complex magnetic structure under the rug and focus on other physical issues. The most common transformation are geometries in which magnetic field lines are straight, i.e. magnetic coordinates.

2.1.1 Covariant and contravariant basis vectors

\{\vec{A}, \vec{B}, \vec{C}\} and \{\vec{a}, \vec{b}, \vec{c}\} are reciprocal iff

\[
\begin{align*}
\vec{A} \cdot \vec{a} &= \vec{B} \cdot \vec{b} = \vec{C} \cdot \vec{c} = 1, \\
\vec{A} \cdot \vec{b} &= \vec{A} \cdot \vec{c} = \vec{B} \cdot \vec{a} = \ldots = 0.
\end{align*}
\]

Any vector \(\vec{P}\) can be written in any of the 2 following ways:

\[
\vec{P} = (\vec{P} \cdot \vec{a})\vec{A} + (\vec{P} \cdot \vec{b})\vec{B} + (\vec{P} \cdot \vec{c})\vec{C},
\]

\[
\vec{P} = (\vec{P} \cdot \vec{A})\vec{a} + (\vec{P} \cdot \vec{B})\vec{b} + (\vec{W} \cdot \vec{C})\vec{c}.
\]

Note that the set of unit basis vectors in Cartesian coordinates \{\(\hat{i}, \hat{j}, \hat{k}\}\} is reciprocal to itself. (\(\hat{i}\)) denotes unit vectors.) Therefore, for both the representations set out in equation (2.1), the components of any position vector \(\vec{P}\) in Cartesian coordinates reads:

\[
\begin{align*}
\vec{P} = x \hat{i} + y \hat{j} + z \hat{k},
\end{align*}
\]

\[
\begin{align*}
x &= \hat{i} \cdot \vec{P}, \\
y &= \hat{j} \cdot \vec{P}, \\
z &= \hat{k} \cdot \vec{P}.
\end{align*}
\]

Suppose that we know the expression of the Cartesian coordinates \((x, y, z)\) in terms of the curvilinear coordinates\(^1\) \((u^1, u^2, u^3)\). Let us define \(\vec{R}\) as the transformation from \((u^1, u^2, u^3)\) to \((x, y, z)\),

\[
\vec{R}(u^1, u^2, u^3) = x(u^1, u^2, u^3) \hat{i} + y(u^1, u^2, u^3) \hat{j} + z(u^1, u^2, u^3) \hat{k}.
\]

\(^1\)i.e curvilinear coordinates are coordinates lines that may be curved and their intersections may form whatever angles
For instance, the transformation from cylindrical coordinates to Cartesian coordinates would be

\[ \vec{R}(r, \theta, z) = r \cos(\theta) \hat{i} + r \sin(\theta) \hat{j} + z \hat{k}. \]  

(2.2)

The differential vector \( d\vec{R} \) can be expressed in terms of \( u^i \). In Einstein notations, it yields

\[ d\vec{R} = \frac{\partial \vec{R}}{\partial u^i} du^i. \]  

(2.3)

And defining the basis vectors

\[ \vec{e}_i = \frac{\partial \vec{R}}{\partial u^i} \]  

(2.4)

that are tangent to the \( u^i \)-curve (curve drawn by \( u^j = \text{constant} \), \( \forall j \neq i \))

\[ d\vec{R} = \vec{e}_i \, du^i \]  

(2.5)

Conversely, \( du^i \) can be written

\[ du^i = (\vec{\nabla}_R \, u^i) \cdot d\vec{R}, \]  

(2.6)

and defining the reciprocal basis vectors

\[ \vec{e}^i = \vec{\nabla}_R \, u^i, \]  

(2.7)

we have

\[ du^i = \vec{e}^i \cdot d\vec{R}. \]  

(2.8)

Indeed, \( \vec{e}^i \) is the reciprocal of \( \vec{e}_i \) as one can infer by combining equations (2.5) and (2.8) that

\[ \vec{e}^i \cdot \vec{e}_j = \delta_{ij}, \]  

(2.9)

where \( \delta_{ij} \) is the Kronecker delta. Note that this implies that reciprocal basis vectors \( \vec{e}^i \) are perpendicular to the coordinate surfaces \( u^i = \text{constant} \).

The relations between covariant and contravariants basis vectors are called cyclic permutations and read

\[ \vec{e}_i = \frac{\vec{e}^j \times \vec{e}^k}{\vec{e}^i \cdot (\vec{e}^j \times \vec{e}^k)}, \]  

(2.10)

with \((i, j, k)\) the cyclic permutations of \((1,2,3)\) i.e. \{\((1,2,3), (3,1,2), (2,3,1)\)\}.

Combining equations (2.1), (2.4) and (2.7) any vector can be defined by its covariant components:

\[ \vec{P} = (\vec{P} \cdot \vec{e}_1) \, \vec{e}_1 + (\vec{P} \cdot \vec{e}_2) \, \vec{e}_2 + (\vec{P} \cdot \vec{e}_3) \, \vec{e}_3, \]  

(2.11)

or its contravariant components:

\[ \vec{P} = (\vec{P} \cdot \vec{e}^1) \, \vec{e}_1 + (\vec{P} \cdot \vec{e}^2) \, \vec{e}_2 + (\vec{P} \cdot \vec{e}^3) \, \vec{e}_3, \]  

(2.13)
2.1 Compendium on magnetic coordinates

Figure 2.1: Illustration [1] of a flux surface (blue) associated with a certain value of $\psi$, and some field lines (red) associated with various values of $\alpha$.

2.1.2 Systems of coordinates

In magnetic coordinates $(\psi, \theta, \zeta)$, the magnetic field can be expressed as

$$\vec{B} = \frac{\Psi'_p}{\sqrt{g}} \vec{e}_\theta + \frac{\Psi'_t}{\sqrt{g}} \vec{e}_\zeta,$$

(2.15)

where $\sqrt{g} = \vec{e}_\psi \cdot \vec{e}_\theta \times \vec{e}_\zeta$ is the volume element, $\Psi'_p$ is the derivative with respect to $\psi$ of the poloidal magnetic flux over $2\pi$, and $\Psi'_t$ is the derivative with respect to $\psi$ of the toroidal magnetic flux over $2\pi$.

Using the rotational transform $\iota = \frac{\Psi'_p}{\Psi'_t}$,

$$\vec{B} = \frac{\Psi'_t}{\sqrt{g}} (\vec{e}_\zeta + \iota(\psi) \vec{e}_\theta),$$

(2.16)

and through the use of relations (2.10), this yields

$$\vec{B} = \Psi'_t (\vec{\nabla}\psi \times \vec{\nabla}\theta - \iota(\psi) \vec{\nabla}\psi \times \vec{\nabla}\zeta),$$

$$\iff \vec{B} = \Psi'_t \vec{\nabla}\psi \times \vec{\nabla}(\theta - \iota(\psi)\zeta).$$

(2.17)

This leads to the definition of another system of coordinates: $\{\psi, l, \alpha\}$, where the role of each coordinate can be broken down as follow:

- $\psi$ is the flux surface label that is present in any flux coordinate set;
- $\alpha = \theta - \iota(\psi)\zeta$ designates the field lines i.e. given a flux surface $\psi$, changing the value of $\alpha$ is equivalent to selecting a different field line (cf. Figure 2.1);
- $l$ denotes the arc length traveled along the field line.

In this system of coordinates, (see equation (2.17)) the magnetic field reads

$$\vec{B} = \Psi'_t \vec{\nabla}\psi \times \vec{\nabla}\alpha.$$
2. Theoretical background

2.2 Drift velocities

2.2.1 Perturbation of the kinetic equation

In general the kinetic equation reads

\[ \frac{Df}{Dt} = C[f, f], \]  \hspace{1cm} (2.19)

where \( \frac{D}{Dt} \) is the total derivative, \( f \) is the distribution function of the described species (e.g. electrons, ions) and \( C[f, f] \) is the collision term.

In terms of the variables \( \{ \vec{r}, E, \mu, \gamma, \sigma, t \} \),

\[ \frac{\partial f}{\partial t} + \dot{\vec{r}} \cdot \nabla_{\vec{r}} f + \dot{\gamma} \nabla_{\gamma} f = C[f, f], \]  \hspace{1cm} (2.20)

where \( \vec{r} \) is the guiding center position, \( E = \frac{v^2}{2} + \frac{Ze\phi}{m_i} \) is the total energy, \( \mu = \frac{v_{\perp}}{B} \) is the magnetic moment, \( \gamma \) is the gyrophase and \( \sigma = \frac{|v||}{|v||} \) is a discrete variable that represents the sign of the parallel velocity \( v_{||} \).

As \( E \) is a constant of motion and \( \mu \) is an adiabatic invariant, we have in steady state

\[ \dot{\vec{r}} \cdot \nabla_{\vec{r}} f + \dot{\gamma} \nabla_{\gamma} f = C[f, f]. \]  \hspace{1cm} (2.21)

Let us define the normalized radius

\[ \rho_{si} = \frac{\rho_i}{L} = \frac{v_{ti}}{\Omega_i L_0}, \]

with \( v_{ti} \) the ion thermal velocity, \( \Omega_i \) the ion gyrofrequency and \( L_0 \sim |\nabla (\log B)|^{-1} \) the typical length of variation of the magnetic field.

In a strongly magnetized plasma, \( \rho_{si} \ll 1 \) and the gyromotion is fast compared to the guiding center motion. Therefore the drift-kinetic approach can be used. It consists in averaging the distribution function \( f \), order by order in \( \rho_{si} \), over the fast gyration of particles around magnetic field lines.

Let us call \( f^{gyro} \) the resulting approximation of \( f \). It is found that \( f^{gyro} \) can be divided into 2 scales:

\[ f^{gyro} = f^{nc} + f^{turb}, \]

where \( f^{nc} \) is the neoclassical approximation that describes the physics of larger scale and \( f^{turb} \) the contribution of turbulence due to fluctuations.

From now on we will only take into account the neoclassical contribution and assume that \( f \) is independent of \( \gamma \). (This can be proven to be true to the accuracy required in the rest of this thesis [8].) We also assume that \( f \) is the main ion distribution and that electrons are not involved in the ion drift-kinetic equation. Then, equation (2.21) becomes

\[ \dot{\vec{r}} \cdot \nabla_{\vec{r}} f = C[f, f]. \]  \hspace{1cm} (2.22)

We will also make the assumption of low ion collisionality

\[ \nu_{is} = \frac{\nu_{ii} L_0}{v_{ti}} \ll \rho_{is}, \]

where \( \nu_{ii} \) is the ion-ion collision frequency.
Let us apply perturbation theory on the distribution function.

\[ f = f^{(0)} + f^{(1)} + f^{(2)} + ..., \]

with \( f^{(n)} \sim \rho_n^0 f \).

At first order, by noting that \( \dot{r} = v_{||} \hat{b} + \vec{v}_d \) (where \( v_d \) is the drift velocity), equation (2.22) yields the following system

\[
\begin{align*}
\begin{cases}
 f^{(0)} \rightarrow v_{||} (\hat{b} \cdot \nabla_{\vec{r}} f^{(0)}) = 0; \\
 f^{(1)} \rightarrow v_{||} (\hat{b} \cdot \nabla_{\vec{r}} f^{(1)}) + \vec{v}_d \cdot \nabla_{\vec{r}} f^{(0)} = C[f^{(0)}, f^{(0)}].
\end{cases}
\end{align*}
\]

(2.23)  \hspace{1cm} (2.24)

In coordinates \( \{ \psi, \alpha, l, \mathcal{E}, \mu, \sigma \} \),

\[ \nabla_{\vec{r}} f = (\nabla_{\vec{r}} \psi) \frac{\partial}{\partial \psi} f + (\nabla_{\vec{r}} \alpha) \frac{\partial}{\partial \alpha} f + (\nabla_{\vec{r}} l) \frac{\partial}{\partial l} f. \]

We recognize the reciprocal basis vector as defined in equation (2.7),

\[ \nabla_{\vec{r}} f = \left( \frac{\partial}{\partial \psi} \right) f + \left( \frac{\partial}{\partial \alpha} \right) f + \left( \frac{\partial}{\partial l} \right) f, \]

so that, from identity (2.9)

\[ \hat{b} \cdot \nabla_{\vec{r}} f^{(0)} = \frac{\partial}{\partial l} f, \]

(2.25)

and the system ((2.23), (2.24)) is recast into

\[
\begin{align*}
\begin{cases}
 v_{||} \frac{\partial f^{(0)}}{\partial l} = 0; \\
 v_{||} \frac{\partial f^{(1)}}{\partial l} + \vec{v}_d \cdot \left( \nabla_{\psi} \frac{\partial f^{(0)}}{\partial \psi} + \nabla_{\alpha} \frac{\partial f^{(0)}}{\partial \alpha} + \nabla_{l} \frac{\partial f^{(0)}}{\partial l} \right) = C[f^{(0)}, f^{(0)}].
\end{cases}
\end{align*}
\]

(2.26)  \hspace{1cm} (2.27)

Hence, from equation (2.26), it can be deduced that, to lowest order, \( f \) does not depend on \( l \),

\[ f \approx f^{(0)}(\psi, \alpha, l, \mathcal{E}, \mu). \]

(2.28)

Besides, the component of velocity that is parallel to the field lines \( v_{||} \) is given by

\[ v_{||} = \sigma \sqrt{2(\mathcal{E} - U)}, \]

(2.29)

where \( U = \mu B - \frac{Ze\phi}{m_i} \) is the potential well the particle undergoes, \( \phi(l) \) being the electric potential. \( \mathcal{E} \) and \( U \) are illustrated in figure 2.2.

From equation (2.29), two main orbit topologies, can be identified.

1. Passing particles: When the total energy \( \mathcal{E} \) of a particle is larger than the maximum of the potential well \( U_M \), the parallel velocity \( v_{||} \) does not change sign.

2. Trapped particles: When the total energy \( \mathcal{E} \) of a particle is not sufficient to overcome the potential barrier \( U_M \), the parallel velocity \( v_{||} \) vanishes at bounce points so that particles go back and forth in a closed trajectory.
Passing particles are always well confined, hence we focus on trapped particles. In order to get information on $f^{(0)}$ from equation (2.27), it is needed to get rid of $f^{(1)}$. To do so, we apply the orbit-average to equation (2.27) so that

$$\langle v_{||} \frac{\partial f^{(1)}}{\partial l} \rangle_{\text{orb.}} + \langle \vec{v}_d \cdot \vec{\nabla} \psi \frac{\partial f^{(0)}}{\partial \psi} \rangle_{\text{orb.}} + \langle \vec{v}_d \cdot \vec{\nabla} \alpha \frac{\partial f^{(0)}}{\partial \alpha} \rangle_{\text{orb.}} + \langle \vec{v}_d \cdot \vec{\nabla} l \frac{\partial f^{(0)}}{\partial l} \rangle_{\text{orb.}} = \langle C[f^{(0)}, f^{(0)}] \rangle_{\text{orb.}},$$

(2.30)

where $\langle g \rangle_{\text{orb.}}$ is defined as

$$\langle g \rangle_{\text{orb.}} = \frac{1}{\tau_b} \oint_{\text{orb.}} \frac{dl}{v_{||}} g.$$

Therefore, the first term of equation (2.30) vanishes. Indeed,

$$\langle v_{||} \frac{\partial f^{(1)}}{\partial l} \rangle_{\text{orb.}} = \frac{1}{\tau_b} \oint_{\text{orb.}} \frac{dl}{v_{||}} v_{||} \frac{\partial f^{(1)}}{\partial l},$$

$$= \frac{1}{\tau_b} \left( \int_{l_L}^{l_R} dl \frac{\partial f^{(1)}}{\partial l} + \int_{l_R}^{l_L} dl \frac{\partial f^{(1)}}{\partial l} \right),$$

$$= \frac{1}{\tau_b} \left( [f^{(1)}]_{l_R}^{l_L} + [f^{(1)}]_{l_L}^{l_R} \right) = 0.$$  

(2.31)

The 4th term of equation 2.30 vanishes too as $f^{(0)}$ does not depend on $l$ (cf. eqn. (2.28)). Thus,

$$\langle \vec{v}_d \cdot \vec{\nabla} \psi \rangle_{\text{orb.}} \frac{\partial f^{(0)}}{\partial \psi} + \langle \vec{v}_d \cdot \vec{\nabla} \alpha \rangle_{\text{orb.}} \frac{\partial f^{(0)}}{\partial \alpha} = \langle C[f^{(0)}, f^{(0)}] \rangle_{\text{orb.}}.$$  

(2.32)
2.2 Drift velocities

2.2.2 Relation between drift velocities and the second adiabatic invariant

This section focuses on the derivation and the analysis of the two relations establishing a link between the orbit averaged drift velocity components $\langle \vec{v}_d \cdot \vec{\nabla} \psi \rangle$ and $\langle \vec{v}_d \cdot \vec{\nabla} \alpha \rangle$ and the second adiabatic invariant $J$. The mentioned identities read

$$\langle \vec{v}_d \cdot \vec{\nabla} \psi \rangle = \frac{m_i}{Ze \Psi_i} \frac{1}{\tau_b} \frac{\partial J}{\partial \alpha}.$$  \hfill (2.33)

$$\langle \vec{v}_d \cdot \vec{\nabla} \alpha \rangle = -\frac{m_i}{Ze \Psi_i} \frac{1}{\tau_b} \frac{\partial J}{\partial \psi}.$$  \hfill (2.34)

where $m_i$ and $Z$ are the mass and the atomic number of the ions, respectively, whereas $e$ is the proton charge.

The drift velocity can be split into three contributions:

$$\vec{v}_d = \vec{v}_\kappa + \vec{v}_{\nabla B} + \vec{v}_E,$$  \hfill (2.35)

where $\vec{v}_\kappa + \vec{v}_{\nabla B}$ represent the magnetic drift and $\vec{v}_E$ the $\vec{E} \times \vec{B}$ drift.

The expressions of $\vec{v}_\kappa$, $\vec{v}_{\nabla B}$ and $\vec{v}_E$ are, respectively,

$$\vec{v}_\kappa = \frac{v_\kappa^2}{\Omega_i} \hat{b} \times \hat{\kappa},$$

$$\vec{v}_{\nabla B} = \frac{\mu}{\Omega_i} \hat{b} \times \vec{\nabla} B,$$

$$\vec{v}_E = \frac{1}{B} \hat{b} \times \vec{\nabla} \phi,$$

with $\kappa = \hat{b} \cdot \vec{\nabla} \hat{b}$ being the curvature of the magnetic field line and $\Omega_i = \frac{ZeB}{m_i}$ being the ion gyrofrequency.

Let us project each drift velocity contribution onto $\vec{\nabla} \psi$,

The curvature drift term

$$\vec{v}_\kappa \cdot \vec{\nabla} \psi = \frac{v_\kappa^2}{\Omega_i} (\hat{b} \times \hat{\kappa}) \cdot \vec{\nabla} \psi.$$  \hfill (2.36)

In the magnetic coordinates $(\psi, \alpha, l)$, using equation (2.14), $\hat{\kappa}$ can be written in terms of its contravariant components,

$$\hat{\kappa} = \left( \hat{b} \cdot \vec{\nabla} \hat{b} \right) \cdot \vec{\nabla} \psi + \left( \hat{b} \cdot \vec{\nabla} \hat{b} \right) \cdot \vec{\nabla} \alpha + \left( \hat{b} \cdot \vec{\nabla} \hat{b} \right) \cdot \frac{\partial \hat{r}^2}{\partial l} \vec{\nabla} l.$$  \hfill (2.37)

The longitudinal coordinate $l$ is chosen so that

$$\frac{\partial \hat{r}^2}{\partial l} = \hat{b},$$  \hfill (2.38)

and recalling equation (2.25), $\hat{\kappa}$ becomes

$$\hat{\kappa} = \frac{\partial \hat{b}}{\partial l} \left( \frac{\partial \hat{r}^2}{\partial \psi} \vec{\nabla} \psi + \frac{\partial \hat{r}^2}{\partial \alpha} \vec{\nabla} \alpha + \hat{b} \vec{\nabla} l \right),$$  \hfill (2.39)
and as \( \frac{\partial \hat{b}}{\partial \alpha} \) is perpendicular to \( \hat{b} \), the last term of equation (2.39) vanishes. Thus \( \vec{\kappa} \) reads now

\[
\vec{\kappa} = \frac{\partial \hat{b}}{\partial l} \cdot \frac{\partial \vec{r}}{\partial \psi} \vec{\nabla} \psi + \frac{\partial \hat{b}}{\partial l} \cdot \frac{\partial \vec{r}}{\partial \alpha} \vec{\nabla} \alpha
\]

(2.40)

Substituting the new expression of \( \vec{\kappa} \) into eqn. (2.36), we find:

\[
\vec{v}_\kappa \cdot \vec{\nabla} \psi = \frac{v_\parallel}{\Omega} \left( \hat{b} \times \left( \frac{\partial \hat{b}}{\partial l} \cdot \frac{\partial \vec{r}}{\partial \psi} \vec{\nabla} \psi + \frac{\partial \hat{b}}{\partial l} \cdot \frac{\partial \vec{r}}{\partial \alpha} \vec{\nabla} \alpha \right) \right) \cdot \vec{\nabla} \psi,
\]

(2.41)

The mathematical identity

\[
(\vec{A} \times \vec{B}) \cdot \vec{C} = (\vec{B} \times \vec{C}) \cdot \vec{A}
\]

applied to this case yields:

\[
\left( \hat{b} \times \vec{\nabla} \psi \right) \cdot \vec{\nabla} \psi = \left( \vec{\nabla} \psi \times \vec{\nabla} \psi \right) \cdot \hat{b} = 0.
\]

(2.42)

\[
\left( \hat{b} \times \vec{\nabla} \alpha \right) \cdot \vec{\nabla} \psi = \left( \vec{\nabla} \alpha \times \vec{\nabla} \psi \right) \cdot \hat{b}.
\]

(2.43)

Hence,

\[
\vec{v}_\kappa \cdot \vec{\nabla} \psi = \frac{v_\parallel}{\Omega} \left( \vec{\nabla} \alpha \times \vec{\nabla} \psi \right) \cdot \hat{b} \left( \frac{\partial \hat{b}}{\partial l} \cdot \frac{\partial \vec{r}}{\partial \alpha} \right).
\]

(2.44)

Furthermore, by definition of \( \psi \) and \( \alpha \) (cf. section 2.1.2),

\[
\vec{B} = \Psi_t' (\vec{\nabla} \psi \times \vec{\nabla} \alpha),
\]

(2.45)

so that,

\[
\vec{v}_\kappa \cdot \vec{\nabla} \psi = - \frac{v_\parallel}{\Omega} \frac{B}{\Psi_t'} \left( \frac{\partial \hat{b}}{\partial l} \cdot \frac{\partial \vec{r}}{\partial \alpha} \right).
\]

(2.46)

Using \((fg)' = f'g + fg'\),

\[
\frac{\partial \hat{b}}{\partial l} \cdot \frac{\partial \vec{r}}{\partial \alpha} = \frac{\partial}{\partial l} (\hat{b} \cdot \frac{\partial \vec{r}}{\partial \alpha}) - \hat{b} \cdot \frac{\partial^2 \vec{r}}{\partial l \partial \alpha},
\]

(2.47)

Let us apply equation (2.38) to the second term,

\[
\frac{\partial^2 \vec{r}}{\partial l \partial \alpha} = \frac{\partial \hat{b}}{\partial \alpha}.
\]

Once again, using that \( \frac{\partial \hat{b}}{\partial \alpha} \) is perpendicular to \( \hat{b} \), equation (2.47) yields

\[
\frac{\partial \hat{b}}{\partial l} \cdot \frac{\partial \vec{r}}{\partial \alpha} = \frac{\partial}{\partial l} \left( \hat{b} \cdot \frac{\partial \vec{r}}{\partial \alpha} \right)
\]

Eventually, equation (2.46) is recast into

\[
\vec{v}_\kappa \cdot \vec{\nabla} \psi = - \frac{v_\parallel}{\Omega} \frac{B}{\Psi_t'} \left( \frac{\partial \hat{b}}{\partial l} \cdot \frac{\partial \vec{r}}{\partial \alpha} \right).
\]

(2.48)
2.2 Drift velocities

The grad-B drift term

Let us now do a similar derivation for the other term of the magnetic drift: \( \tilde{v}_{\nabla B} \).

\[
\tilde{v}_{\nabla B} \cdot \nabla \psi = \frac{\mu}{\Omega_i} \left( \hat{b} \times \nabla B \right) \cdot \nabla \psi
\]

Applying the chain rule on \( \nabla B \) gives

\[
\nabla B = \frac{\partial B}{\partial \psi} \nabla \psi + \frac{\partial B}{\partial \alpha} \nabla \alpha + \frac{\partial B}{\partial l} \nabla l.
\] (2.49)

Hence, as \( (\hat{b} \times \nabla \psi) \cdot \nabla \psi = 0 \),

\[
\tilde{v}_{\nabla B} \cdot \nabla \psi = \frac{\mu}{\Omega_i} \left( \hat{b} \times \left( \frac{\partial B}{\partial \alpha} \nabla \alpha + \frac{\partial B}{\partial l} \nabla l \right) \right) \cdot \nabla \psi
\]

\[
= \frac{\mu}{\Omega_i} \left( \frac{\partial B}{\partial \alpha} (\hat{b} \times \nabla \alpha) \cdot \nabla \psi + \frac{\partial B}{\partial l} (\hat{b} \times \nabla l) \cdot \nabla \psi \right)
\]

\[
= \frac{\mu}{\Omega_i} \left( - \frac{\partial B}{\partial \alpha} B \Psi' t \nabla \alpha \cdot \hat{b} - \frac{\partial B}{\partial l} (\nabla l \times \nabla \psi) \cdot \hat{b} \right),
\]

where the last equality was found using equations (2.43) and (2.45).

Let us use cyclic permutations (cf. section 2.1.1) to express the quantity \( \nabla l \times \nabla \psi \) in a more convenient way. By definition, \( \hat{e}_i = \frac{\partial r}{\partial u_i} \) and \( \hat{e}^i = \nabla u^i \). Thus equation (2.10) writes as follow in the system of coordinates \( \{ \psi, \alpha, l \} \),

\[
\frac{\partial r}{\partial \alpha} = \frac{\nabla l \times \nabla \psi}{\nabla \alpha \cdot (\nabla l \times \nabla \psi)},
\]

which, using eqn. (2.41) and (2.45), can be changed into

\[
\frac{\partial r}{\partial \alpha} = \frac{\nabla l \times \nabla \psi}{B/\Psi' t \nabla l \cdot \hat{b}},
\]

Moreover, as \( \nabla l \cdot \hat{b} = 1 \)

\[
\nabla l \times \nabla \psi = \frac{B}{\Psi' t} \frac{\partial r}{\partial \alpha},
\] (2.50)

and finally,

\[
\tilde{v}_{\nabla B} \cdot \nabla \psi = \frac{\mu}{\Omega_i} \frac{B}{\Psi' t} \left( - \frac{\partial B}{\partial \alpha} + \frac{\partial B}{\partial l} \frac{\partial r}{\partial \alpha} \cdot \hat{b} \right).
\] (2.51)

The \( \vec{E} \times \vec{B} \) drift term

The last contribution of the drift velocity to be computed is the one associated with the \( \vec{E} \times \vec{B} \) drift, \( \tilde{v}_E \).

\[
\tilde{v}_E \cdot \nabla \psi = \frac{1}{B} (\hat{b} \times \nabla \phi) \cdot \nabla \psi
\]

Exactly through the same process as for the \( \tilde{v}_{\nabla B} \cdot \nabla \psi \) term, it is found that

\[
\tilde{v}_E \cdot \nabla \psi = \frac{1}{\Psi' t} \left( - \frac{\partial \phi}{\partial \alpha} + \frac{\partial \phi}{\partial l} \frac{\partial r}{\partial \alpha} \cdot \hat{b} \right).
\] (2.52)
Derivation of relations (2.33) and (2.34)

- Gathering equations (2.36), (2.51) and (2.52),

\[
\vec{v}_d \cdot \nabla \psi = \left( -\frac{v_\parallel^2}{\Omega_i} B \frac{\partial}{\partial l} \left( \hat{b} \cdot \frac{\partial \vec{r}}{\partial \alpha} \right) \right) + \left( \frac{\mu_i}{\Omega_i} \frac{B}{\Psi_i} \left( -\frac{\partial B}{\partial \alpha} + \frac{\partial B}{\partial l} \frac{\partial}{\partial \alpha} \hat{b} \right) \right) + \left( \frac{1}{\Psi_i} \left( -\frac{\partial \phi}{\partial \alpha} + \frac{\partial \phi}{\partial l} \frac{\partial}{\partial \alpha} \hat{b} \right) \right),
\]

(2.53)

so that, by integrating over \( l \) and developing \( \Omega_i \) into \( \frac{ZeB}{m_i} \)

\[
2 \int_{l_L}^{l_R} dl \frac{\vec{v}_d}{|v_\parallel|} \cdot \nabla \psi = 2 \int_{l_L}^{l_R} dl \left( -\frac{v_\parallel m_i}{Ze \Psi_i} \frac{B}{\Psi_i} \frac{\partial}{\partial l} \left( \hat{b} \cdot \frac{\partial \vec{r}}{\partial \alpha} \right) \right)
+ 2 \int_{l_L}^{l_R} dl \frac{m_i}{Ze|v_\parallel|\Psi_i} \left( -\frac{\partial}{\partial \alpha} \mu B - \frac{\partial}{\partial l} \mu B \frac{\partial \vec{r}}{\partial \alpha} \hat{b} \right)
+ 2 \int_{l_L}^{l_R} dl \frac{m_i}{Ze|v_\parallel|\Psi_i} \left( -\frac{\partial}{\partial \alpha} Ze \phi m_i - \frac{\partial}{\partial l} Ze \phi \frac{\partial \vec{r}}{\partial \alpha} \hat{b} \right). \tag{2.54}
\]

Hence, by definition of the orbit average,

\[
\langle \vec{v}_d \cdot \nabla \psi \rangle = \frac{2m_i}{Ze \Psi_i} \frac{1}{\tau_b} \int_{l_L}^{l_R} dl \left( -\frac{v_\parallel}{|v_\parallel|} \frac{\partial}{\partial l} \left( \hat{b} \cdot \frac{\partial \vec{r}}{\partial \alpha} \right) \right)
+ \frac{2m_i}{Ze \Psi_i} \frac{1}{\tau_b} \int_{l_L}^{l_R} dl \left( -\frac{1}{|v_\parallel|} \left( -\frac{\partial}{\partial \alpha} \mu B + \frac{\partial}{\partial l} \mu B \frac{\partial \vec{r}}{\partial \alpha} \hat{b} \right)
- \left( \frac{\partial}{\partial \alpha} Ze \phi m_i + \frac{\partial}{\partial l} Ze \phi \frac{\partial \vec{r}}{\partial \alpha} \hat{b} \right) \right), \tag{2.55}
\]

and rearranging the terms,

\[
\langle \vec{v}_d \cdot \nabla \psi \rangle = -\frac{2m_i}{Ze \Psi_i} \frac{1}{\tau_b} \int_{l_L}^{l_R} dl \frac{v_\parallel}{|v_\parallel|} \frac{\partial}{\partial l} \left( \hat{b} \cdot \frac{\partial \vec{r}}{\partial \alpha} \right)
+ \frac{2m_i}{Ze \Psi_i} \frac{1}{\tau_b} \int_{l_L}^{l_R} dl \frac{1}{|v_\parallel|} \left( -\frac{\partial}{\partial \alpha} \left( \mu B + \frac{Ze \phi}{m_i} \right) \right)
+ \frac{\partial}{\partial l} \left( \mu B + \frac{Ze \phi}{m_i} \right) \frac{\partial \vec{r}}{\partial \alpha} \hat{b}. \tag{2.56}
\]

- By using the definition of \( E \) and \( \mu \), it is found that

\[
\mu B + \frac{Ze \phi}{m_i} = E - \frac{v_\parallel^2}{2} \tag{2.57}
\]

As \( E, \alpha \) and \( l \) are independent variables, the derivatives of \( E \) with regard to \( \alpha \) and \( l \) both vanish so that equation (2.56) can be recast into

\[
\langle \vec{v}_d \cdot \nabla \psi \rangle = \frac{2m_i}{Ze \Psi_i} \frac{1}{\tau_b} \int_{l_L}^{l_R} dl \left( -v_\parallel \frac{\partial}{\partial l} \left( \hat{b} \cdot \frac{\partial \vec{r}}{\partial \alpha} \right) + \frac{\partial v_\parallel}{\partial \alpha} - \frac{\partial v_\parallel}{\partial l} \frac{\partial \vec{r}}{\partial \alpha} \hat{b} \right). \tag{2.58}
\]
The product rule yields
\[ v_{||} \frac{\partial}{\partial l} (\dot{b} \cdot \frac{\partial \vec{r}}{\partial \alpha}) + \frac{\partial v_{||}}{\partial l} \frac{\partial \vec{r}}{\partial \alpha} \cdot \ddot{b} = \frac{\partial}{\partial l} (v_{||} \dot{b} \cdot \frac{\partial \vec{r}}{\partial \alpha}). \quad (2.59) \]

Therefore, equation (2.58) is simplified into
\[ \langle \vec{v}_d \cdot \vec{\nabla} \psi \rangle = \frac{2m_i}{Ze\Psi_t} \frac{1}{\tau_b} \frac{\partial J}{\partial \alpha} \int_{l_{\text{L}}}^{l_{\text{R}}} dl \ v_{||} - \frac{2m_i}{Ze\Psi_t} \int_{l_{\text{L}}}^{l_{\text{R}}} dl \frac{\partial}{\partial l} (v_{||} \dot{b} \cdot \frac{\partial \vec{r}}{\partial \alpha}). \quad (2.60) \]

In the first term on the right-hand side, we recognize the second adiabatic invariant \( J = 2 \int_{l_{\text{L}}}^{l_{\text{R}}} dl \ v_{||} \), and as \( v_{||} \) vanishes at the endpoints of the integral, the second term on the right-hand side vanishes. Then,
\[ \langle \vec{v}_d \cdot \vec{\nabla} \psi \rangle = \frac{m_i}{Ze\Psi_t} \frac{1}{\tau_b} \frac{\partial J}{\partial \alpha}. \quad (2.61) \]

Analogously, one can show that
\[ \langle \vec{v}_d \cdot \vec{\nabla} \alpha \rangle = -\frac{m_i}{Ze\Psi_t} \frac{1}{\tau_b} \frac{\partial J}{\partial \psi}. \quad (2.62) \]

Furthermore, similarly to what was done to derive equation (2.32), the material derivative of \( J \) can be expressed as
\[ \frac{dJ}{dt} = \langle \vec{v}_d \cdot \vec{\nabla} \psi \rangle_{\text{orb.}} \frac{\partial J}{\partial \psi} + \langle \vec{v}_d \cdot \vec{\nabla} \alpha \rangle_{\text{orb.}} \frac{\partial J}{\partial \alpha}. \tag{2.63} \]

Substituting equations (2.61) and (2.62) into equation (2.63) yields
\[ \frac{dJ}{dt} = 0, \tag{2.64} \]
from which it can be inferred that trapped particles follow trajectories of constant \( J \). Moreover, from equation (2.61), it can be deduced that a magnetic configuration is omnigeneous if and only if
\[ \frac{\partial J}{\partial \alpha} = 0. \tag{2.65} \]
2. Theoretical background

Figure 2.3: Illustration of the magnetic well in which the particle is trapped. The bounce points $l_L, l_R$ and the cordinate $\tilde{B}$ are depicted.

2.3 From $J(B)$ to $B(J)$

Let us now consider the motion of a trapped particle in a simple magnetic well as illustrated in figure 2.3, the second adiabatic invariant $J$ can be expressed as

$$J = 2 \int_{l_L}^{l_R} dl |v||. \quad (2.66)$$

We use the pitch angle $\lambda = v_\perp^2 / (v^2 B)$ as the velocity coordinate alongside with the velocity magnitude $v$. In coordinates $(\psi, \alpha, l, \lambda, v)$, equation (2.66) becomes

$$J(\psi, \alpha, \lambda, v) = 2v \int_{l_L(\psi, \alpha, \lambda)}^{l_R(\psi, \alpha, \lambda)} dl \sqrt{1 - \lambda B(\psi, \alpha, l)}. \quad (2.67)$$

If the configuration is omnigeneous, equation (2.65) states that $J$ is independent of $\alpha$ even though the endpoints of the integral and the integrand do depend on $\alpha$. From now on, to make the notation less cluttered, we drop the dependency on $\psi$ and $\alpha$.

As $l_L$ and $l_R$ are the bounce points of the trapped orbits at which $v|$ vanishes, it follows that

$$\begin{cases} 1 - \lambda B(l_L) = 0, \\ 1 - \lambda B(l_R) = 0, \end{cases} \quad (2.68)$$

which sets the accessible range of $\lambda$ to $[B_{\text{max}}^{-1}, B_{\text{min}}^{-1}]$ for trapped particles.

2.3.1 Derivation of $B(J)$

What follows is the derivation of Cary and Sasharina’s expression [10] through the inversion of equation (2.67). Doing so, together with some constraints, provides the magnetic field spatial distribution as a function of the second adiabatic invariant i.e. $B(J)$.
Let us use \( \tilde{B} \in [B_{\text{min}}, B_{\text{max}}] \), the strength of the magnetic field at which our particle is reflected i.e. \( \tilde{B} = B(l_L) = B(l_R) \), as coordinate. and divide equation (2.67) by \( \sqrt{\lambda B - 1} \),

\[
\frac{\tilde{J}(\lambda)}{\sqrt{\lambda B - 1}} = 2 \int_{l_L(\lambda)}^{l_R(\lambda)} dl \frac{\sqrt{1 - \lambda B(l)}}{\sqrt{\lambda B - 1}},
\]  

(2.69)

where we have introduced \( \tilde{J}(\lambda) = \frac{J(v, \lambda)}{B} \).

We now integrate over \( \lambda \) from \( [\tilde{B}^{-1} \text{ to } B_{\text{min}}^{-1}] \),

\[
\int_{\tilde{B}^{-1}}^{B_{\text{min}}^{-1}} d\lambda \frac{\tilde{J}(\lambda)}{\sqrt{\lambda B - 1}} = 2 \int_{l_L(\tilde{B}^{-1})}^{l_R(\tilde{B}^{-1})} dl \int_{\tilde{B}^{-1}}^{B^{-1}} d\lambda \frac{\sqrt{1 - \lambda B(l)}}{\sqrt{\lambda B - 1}}.
\]  

(2.70)

The order of the double integral on the right-hand side can be inverted. The bounds of the integral are to be adapted consequently as depicted in figures 2.4 and 2.5. This process yields

\[
\int_{B_{\text{min}}^{-1}}^{\tilde{B}^{-1}} d\lambda \frac{\tilde{J}(\lambda)}{\sqrt{\lambda B - 1}} = 2 \int_{l_L(\tilde{B}^{-1})}^{l_R(\tilde{B}^{-1})} dl \int_{\tilde{B}^{-1}}^{B^{-1}} d\lambda \frac{\sqrt{1 - \lambda B(l)}}{\sqrt{\lambda B - 1}}.
\]  

(2.71)

The right-hand side integrand is recast into

\[
2 \int_{l_L(\tilde{B}^{-1})}^{l_R(\tilde{B}^{-1})} dl \sqrt{\frac{B(l)}{\tilde{B}}} \int_{\tilde{B}^{-1}}^{B^{-1}} d\lambda \sqrt{\frac{B^{-1}(l) - \lambda}{B^{-1}(l) - \tilde{B}^{-1}}}.
\]

Using identity

\[
\int_a^b dx \sqrt{\frac{b - x}{x - a}} = \frac{\pi}{2} (b - a),
\]

(2.72)
equation (2.71) reads

\[
\int_{B_{\text{min}}^{-1}}^{\tilde{B}^{-1}} d\lambda \frac{\tilde{J}(\lambda) \sqrt{\tilde{B}}}{\sqrt{\lambda B - 1}} = \pi \int_{l_L(\tilde{B}^{-1})}^{l_R(\tilde{B}^{-1})} dl \sqrt{\frac{B(l)}{\tilde{B}}} \left( B^{-1}(l) - \tilde{B}^{-1} \right).
\]

(2.73)

By defining \( \Xi(l, \tilde{B}^{-1}) = \sqrt{\frac{B(l)}{\tilde{B}}} \left( B^{-1}(l) - \tilde{B}^{-1} \right) \), equation (2.73) can be written as

\[
\int_{B_{\text{min}}^{-1}}^{\tilde{B}^{-1}} d\lambda \frac{\tilde{J}(\lambda) \sqrt{\tilde{B}}}{\sqrt{\lambda B - 1}} = \pi \int_{l_L(\tilde{B}^{-1})}^{l_R(\tilde{B}^{-1})} dl \Xi(l, \tilde{B}^{-1}).
\]

(2.74)

Differentiating the right-hand side of equation (2.74) with respect to \( \tilde{B}^{-1} \) according to Leibniz’s integral rule yields

\[
\frac{\partial}{\partial \tilde{B}^{-1}} \int_{l_L(\tilde{B}^{-1})}^{l_R(\tilde{B}^{-1})} dl \Xi = \Xi \bigg|_{l=l_R} \frac{dl_R}{d\tilde{B}^{-1}} - \Xi \bigg|_{l=l_L} \frac{dl_L}{d\tilde{B}^{-1}} + \int_{l_L(\tilde{B}^{-1})}^{l_R(\tilde{B}^{-1})} dl \frac{\partial \Xi}{\partial \tilde{B}^{-1}},
\]

with

\[
\begin{align*}
\Xi \bigg|_{l=l_R} &= 0, \\
\Xi \bigg|_{l=l_L} &= 0, \\
\frac{\partial \Xi}{\partial \tilde{B}^{-1}} &= -\sqrt{B(l)}.
\end{align*}
\]

(2.75)
2. Theoretical background

Figure 2.4: Domain of integration for the double integral of equation (2.70). The integrand is firstly integrated over \( l \) from \( l_L(\lambda) \) to \( l_R(\lambda) \) as depicted by each green vertical line. Each line is associated with a value of \( \lambda \in [\tilde{B}^{-1}, B_{min}^{-1}] \) which define the bounds of the integral over \( \lambda \).

Figure 2.5: Domain resulting from reversing the integration order. The integrand is firstly integrated over \( \lambda \) from \( \tilde{B}^{-1} \) to \( \lambda(l_B) \) as depicted by each green horizontal line. From equation (2.68), it can be inferred that \( \lambda(l_B) = B^{-1} \). Each line is associated with a value of \( l \) in the range \([l_L(\tilde{B}^{-1}), l_R(\tilde{B}^{-1})]\) as the extrema of \( l_L \) and \( l_R \) are reached at \( \lambda = \tilde{B}^{-1} \).
Thus, the differentiation yields

\[
\frac{\partial}{\partial \tilde{B}^{-1}} \int_{\tilde{B}^{-1}}^{B_{\text{min}}^{-1}} d\lambda \frac{\tilde{J}(\lambda) \sqrt{\tilde{B}}}{\sqrt{\lambda \tilde{B} - 1}} = -\pi \int_{l_{\text{L}}(\tilde{B}^{-1})}^{l_{\text{R}}(\tilde{B}^{-1})} dl \sqrt{B(l)}. \quad (2.76)
\]

We take the derivative with regard to $\tilde{B}^{-1}$ of equation (2.76)

\[
\frac{\partial^2}{\partial (\tilde{B}^{-1})^2} \int_{B_{\text{min}}^{-1}}^{B_{\text{max}}^{-1}} d\lambda \frac{\tilde{J}(\lambda) \sqrt{\tilde{B}}}{\sqrt{\lambda \tilde{B} - 1}} = -\pi \left( \sqrt{B(l_{\text{R}})} \frac{\partial l_{\text{R}}}{\partial \tilde{B}^{-1}} - \sqrt{B(l_{\text{L}})} \frac{\partial l_{\text{L}}}{\partial \tilde{B}^{-1}} \right). \quad (2.77)
\]

Let us call $l_{B} = \{l_{L}, l_{R}\}$. Expression $B^{-1}(l_{B}) = \tilde{B}^{-1}$ can be differentiated with regard to $\tilde{B}^{-1}$,

\[
1 = \frac{\partial B^{-1}}{\partial l} \bigg|_{l = l_{B}} \frac{\partial l_{B}}{\partial \tilde{B}^{-1}} = -B^{-2}(l_{B}) \frac{\partial B}{\partial l} \bigg|_{l = l_{B}} \frac{\partial l_{B}}{\partial \tilde{B}^{-1}}, \quad (2.78)
\]

which yields

\[
\frac{\partial l_{B}}{\partial \tilde{B}^{-1}} = -\tilde{B}^{2} \left( \frac{\partial B}{\partial l} \right)^{-1} \bigg|_{l = l_{B}}. \quad (2.79)
\]

By substituting equation (2.79) into equation (2.77), it is found that

\[
\frac{\partial^2}{\partial (\tilde{B}^{-1})^2} \int_{B^{-1}}^{B_{\text{min}}^{-1}} d\lambda \frac{\tilde{J}(\lambda) \sqrt{\tilde{B}}}{\sqrt{\lambda \tilde{B} - 1}} = \pi \left( \sqrt{\tilde{B}} \tilde{B}^2 \left( \frac{\partial B}{\partial l} \right)^{-1} \bigg|_{l = l_{R}} - \sqrt{\tilde{B}} \tilde{B}^2 \left( \frac{\partial B}{\partial l} \right)^{-1} \bigg|_{l = l_{L}} \right). \quad (2.80)
\]

Finally,

\[
\left( \frac{\partial B}{\partial l} \right)^{-1} \bigg|_{l = l_{R}} - \left( \frac{\partial B}{\partial l} \right)^{-1} \bigg|_{l = l_{L}} = \frac{1}{\pi B^{5/2}} \frac{\partial^2}{\partial (\tilde{B}^{-1})^2} \left( \int_{B^{-1}}^{B_{\text{min}}^{-1}} d\lambda \frac{\tilde{J}(\lambda) \sqrt{\tilde{B}}}{\sqrt{\lambda \tilde{B} - 1}} \right). \quad (2.81)
\]

Using this equation, for a given magnetic field line, i.e. for fixed values of $\alpha$ and $\psi$, permits one to get the omnigeneous equivalent of the right side of the magnetic well (red curve in figure 2.3), characterized by $\left( \frac{\partial B}{\partial l} \right)^{-1} \bigg|_{l = l_{R}}$, into which a particle is trapped. The required inputs are the left side of the well (blue curve in figure 2.3), i.e. $\left( \frac{\partial B}{\partial l} \right)^{-1} \bigg|_{l = l_{L}}$, and the second adiabatic invariant $J$.

This is the final result of this chapter, we will use equation (2.81) throughout the rest of this document.
2. Theoretical background
Chapter 3

Methodology of the simulation

In section 2.3.1, we obtained
\[
\left( \frac{\partial B}{\partial l} \right)^{-1} \bigg|_{l=l_R} - \left( \frac{\partial B}{\partial l} \right)^{-1} \bigg|_{l=l_L} = \frac{1}{\pi v B^{5/2}} \frac{\partial^2}{\partial (B^{-1})^2} \left( \int_{B^{-1}}^{B^{-1}_{\min}} d\lambda \frac{J(\lambda) \sqrt{B}}{\sqrt{\lambda B - 1}} \right),
\]
(3.1)

where \( l_L \) and \( l_R \) are the bounce points on the left side and right side of the magnetic well, respectively. \( B_{\min} \) and \( B_{\max} \) are the minimum and maximum values of the magnetic field strength inside the well and \( \tilde{B} \) is included in the interval \([B_{\min}, B_{\max}]\). These quantities are depicted in figure 2.3.

The well can be expressed as \( B(l) \) or \( l(B) \) indistinctly. As the right-hand side of equation (3.1) was defined as a function of \( \tilde{B}^{-1} \), the \( l(B) \) representation was found to be more convenient. Indeed, in this context, \( B \) can be chosen as an array going from the minimum value of the magnetic well to its highest value, \( B_{\min} \) and \( B_{\max} \) respectively, with a constant spacing \( \Delta B \).

In coordinates \((\psi, \alpha, l)\), the magnetic well is delimited by \( l_L(B_{\max}) \) and \( l_R(B_{\max}) \) that are provided by the boundary conditions:

\[
\begin{aligned}
\left. \frac{\partial B}{\partial l} \right|_{l=l_L(B_{\max})} &= 0, \\
\left. \frac{\partial B}{\partial l} \right|_{l=l_R(B_{\max})} &= 0,
\end{aligned}
\]
(3.2)

The part of the magnetic field that is used as an input is the left side of the well defined as \( l_L(B) \) whereas the output is the right side of the well, namely \( l_R(B) \), with \( B \in [B_{\min}, B_{\max}] \). These two parts connect at the bottom of the well as illustrated in figure 2.3. This section describes how the right part of the well was obtained through the implementation of equation (2.81) in FORTRAN 90 language whereas the results are described in Chapter 4.

Firstly, the quantity \( \tilde{J} = \frac{J(\lambda)}{v} \) was computed numerically from equation (2.67) using \( B(\theta, \zeta) \) as an input. Then the computation of the right-handside integral of equation (3.1) was tackled. In order to do so, we applied a grid uniform in \( \tilde{B}^{-1} \), and use a generalized midpoint rule as the integrand is not defined at its lower boundary (i.e. \( \lambda = \tilde{B}^{-1} \)). The algorithm "midpnt" from [11] showed to be sufficient. An archetype of the method is illustrated in figure 3.1.
3. Methodology of the simulation

Figure 3.1: Paradigm of the midpoint method illustrated (picture from http://tutorial.math.lamar.edu/Classes/CalcII/ApproximatingDefIntegrals.aspx).

Let us call $I$ the above-mentioned integral, the second derivative of $I$ with respect to $\tilde{B}^{-1}$ was computed based on the centered finite difference formula

$$\frac{\partial^2 I}{\partial (\tilde{B}^{-1})^2} \approx \frac{I(\tilde{B}_{i+1}^{-1}) - 2I(\tilde{B}_i^{-1}) + I(\tilde{B}_{i-1}^{-1})}{(\Delta \tilde{B}^{-1})^2},$$  \hspace{1cm} (3.3)

where $\Delta \tilde{B}^{-1} = \tilde{B}_{i+1}^{-1} - \tilde{B}_i^{-1}$ is the spacing of the grid. At that point, the final grid was set, that is a grid uniform with respect to $B$. Thus the spacing $\Delta B = B_{i+1} - B_i$ is constant from now on.

Let $\Upsilon(\tilde{B}^{-1})$ be the right-hand side of the equation (3.1), it rewrites into

$$\left( \frac{\partial B}{\partial l} \right)_{l=I_L(\tilde{B})}^{l=I_R(\tilde{B})} = \Upsilon(\tilde{B}^{-1}).$$ \hspace{1cm} (3.4)

Besides, the magnetic field strength used as an input was provided in Boozer coordinates $(\psi, \theta, \zeta)$. Therefore, let us use Boozer coordinates from now on. In this context, fixing $\alpha$, results in setting a constraint on the variation of one toroidal flux angles ($\theta$ and $\zeta$) with respect to the other. Indeed, as seen in section 2.1.2, $\alpha = \theta - \iota(\psi)\zeta$. Thus, for a fixed value of $\alpha$, the derivatives with regard to $l$ are expressed the following way

$$\frac{\partial B(l)}{\partial l} = \frac{\partial B(\zeta)}{\partial \zeta} \frac{d \zeta}{dl},$$ \hspace{1cm} (3.5)

and equation (3.4) becomes:

$$\left( \frac{\partial B}{\partial \zeta} \right)_{\zeta(I_R)}^{l=I_L(\tilde{B})} - \left( \frac{\partial B}{\partial \zeta} \right)_{\zeta(I_L)}^{l=I_R(\tilde{B})} = \hat{\Upsilon}(\tilde{B}^{-1}),$$ \hspace{1cm} (3.6)

where $\hat{\Upsilon} = \frac{d\zeta}{dl} \bigg|_{l(\tilde{B})} \Upsilon(\tilde{B}^{-1})$ and $\frac{d\zeta}{dl}$ was provided as an input.

The mathematical expression (3.6) can be discretized into

$$\left( \frac{\Delta B}{\zeta(I_R(\tilde{B}_{i+1})) - \zeta(I_R(\tilde{B}_i))} \right)^{-1} - \left( \frac{\Delta B}{\zeta(I_L(\tilde{B}_{i+1})) - \zeta(I_L(\tilde{B}_i))} \right)^{-1} = \hat{\Upsilon}(\tilde{B}_i^{-1}).$$
Let us use the notation $\zeta^i_{R} = \zeta(l_R(\tilde{B}_i))$, the previous expression becomes
\[
\left( \frac{\Delta B}{\zeta^{i+1}_{R} - \zeta^i_{R}} \right)^{-1} - \left( \frac{\Delta B}{\zeta^{i+1}_{L} - \zeta^i_{L}} \right)^{-1} = \tilde{\Upsilon}(\tilde{B}_i^{-1}),
\]
which yields
\[
\zeta^{i+1}_{R} = \zeta^{i}_{R} + \zeta^{i+1}_{L} - \zeta^{i}_{L} + \tilde{\Upsilon}(\tilde{B}_i^{-1}) \Delta B, \tag{3.7}
\]
with the initial condition $\zeta^1_{R} = \zeta^1_{L}$. The quantities present in equation (3.7) are illustrated in figure 3.2.
3. Methodology of the simulation
Chapter 4

Results

4.1 Studied configurations

The flux surfaces ($\psi$ fixed) of two different magnetic configurations were investigated. Each one of the two was provided in Boozer magnetic flux coordinates,

$$B(\theta, \zeta) = \sum_{m=0}^{\infty} \sum_{n=-\infty}^{\infty} b_{m,n} \cos(m\theta + Nn\zeta),$$  

(4.1)

where $m$ and $n$ are respectively the poloidal and toroidal modes, $N$ is the field period number. In both cases $N = 4$.

The first one to be considered was a flux surface of an ideal quasisymmetric configuration. This was achieved by selecting the two largest Fourier modes of the magnetic configuration of HSX and removing the others. The direction of symmetry can clearly be identified in figure 4.1a where both the magnetic field and the curve $\alpha = 0$ are represented. The magnetic strength along this field line is sinusoidal in $\zeta$ as illustrated in figure 4.3a.

The second configuration that was studied was omnigenous but not quasisymmetric. In this case, there is no direction of symmetry that can be identified, and the magnetic configuration along a fieldline is not a simple sinus. The magnetic field is depicted in figure 4.1b in terms of Boozer angles while the magnetic strength along the fieldline $\alpha = 0$ is shown in figure 4.3b. This configuration was created based on a method proposed by Landreman in [12].

4.2 Numerical results

In this section, we reconstitute, for each configuration, one of the magnetic wells located along the field line $\alpha = 0$ (cf. figure 4.3).

In figure 4.2 are the solutions of equation (2.67), that yields the second adiabatic invariant as a function of the pitch angle $\lambda$, both for the quasi-symmetric and the omnigenous case. It can be observed that $J$ vanishes as expected at

$$\lambda = 1/B_{\text{min}},$$

since at the bottom of the well, trapped particles have orbits of zero size.

The reconstitution of the magnetic well for both the quasisymmetric and omnigenous configurations is illustrated in figures 4.3 and 4.4. It can be observed in the former
4. Results

(a) Quasi-symmetric configuration.

(b) Omnigeneous configuration.

Figure 4.1: Contour plots of the studied magnetic configurations in Boozer coordinates ($\psi$ fixed), that is the magnetic field strength as a function of the angular coordinates $\theta$ and $\zeta$. The curves $\alpha = 0$ are also represented (in dark).

Figure 4.2: Normalized second adiabatic invariant as a function of $\lambda$ as calculated using equation (2.67) for the quasisymmetric and the omnigeneous magnetic configurations. Note that $\lambda_{\text{min}} = 1/B_{\text{max}}$ and $\lambda_{\text{max}} = 1/B_{\text{min}}$. 
### 4.2 Numerical results

#### Figure 4.3: Magnetic field along the field line $\alpha = 0$ as a function of the toroidal coordinate $\zeta$ (in red) and numerical reconstitution of the magnetic well (in green).

(a) Quasi-symmetric configuration.  
(b) Omnigeneous configuration.

#### Figure 4.4: Close-up of the magnetic well shown in figure 4.3 in both the quasisymmetric and the omnigeneous case.

(a) Quasi-symmetric configuration.  
(b) Omnigeneous configuration.

that the constructed well fits perfectly the configuration on which it is based. Indeed, the reconstituted magnetic well (plotted in green) matches the magnetic configuration (plotted in red). The left part of the well was provided as an input while the right part was calculated following the explanations provided in section 3. It can be seen from figure 4.4 that the two halves smoothly connect at the bottom of the well.

The simulations were also successfully performed for different values of $\alpha$, which is equivalent to choosing a different field line as illustrated for the omnigeneous configuration in figure 4.5. The magnetic field along the field line $\alpha = 2$ is depicted in figure 4.6 whereas it can be inferred from figure 4.1a that, in the quasisymmetric configuration, changing the value of alpha is equivalent to introducing a shift in $\zeta$.

Eventually it can be observed in figure 4.7 that we do not find the same well as in figure 4.4b. Therefore, the shape of omnigeneous magnetic configurations generally depends on $\alpha$ while it does not for quasisymmetric configurations.
4. Results

Figure 4.5: Contour plot of the studied magnetic configurations on which both the curves $\alpha = 0$ and $\alpha = 2$ are represented (in dark).

Figure 4.6: Magnetic field along the field line $\alpha = 2$ as a function of the toroidal coordinate $\zeta$ (in red) and numerical reconstitution of the magnetic well (in green).

Figure 4.7: Reconstitution of the magnetic well in the omnigeneous case for $\alpha = 2$. 
Chapter 5

Conclusions

Some analytical and numerical tools that can be used to describe perfectly optimized stellarators were tested in this work. The theoretical background necessary for the understanding of stellarator optimization with respect to radial neoclassical transport was therewith briefly presented.

In particular, we deduced, by applying perturbation theory on the neoclassical kinetic equation at low collisionalities, that at zeroth order the distribution function does not depend on the longitudinal coordinate $l$, i.e. the particle distribution does not vary along field lines.

The derivation of the relations between the drift velocity and the second adiabatic invariant \[<\vec{v}_d \cdot \vec{\nabla} \psi> = \frac{m_i}{Ze} \frac{1}{\tau_b} \frac{\partial J}{\partial \alpha}, \quad (5.1)\]
was detailed and we saw that, from these relations, it can be inferred that since particles follow trajectories that conserve the second adiabatic invariant, optimized stellarators must satisfy the condition \[\frac{\partial J}{\partial \alpha} = 0. \quad (5.2)\]

The derivation of Cary’s equation

\[
\left( \frac{\partial B}{\partial l} \right)^{-1} \bigg|_{l=l_L} - \left( \frac{\partial B}{\partial l} \right)^{-1} \bigg|_{l=l_R} = \frac{1}{\pi v B^{5/2}} \frac{\partial^2}{\partial (B^{-1})^2} \left( \int_{B^{-1}}^{B_{\text{min}}} d\lambda \frac{J(\lambda) \sqrt{B}}{\sqrt{\lambda B - 1}} \right), \quad (5.3)
\]
was revisited and the expression was then numerically implemented. By doing so, it was possible, provided the value of the magnetic field strength on (roughly) half a flux-surface of an omnigeneous stellarator, to determine its counterpart on the rest of it, and this for two different magnetic configurations.

The resulting reconstitution of the magnetic configurations was successfully done for multiple field lines which allowed us to observe that, in omnigeneous stellarators, the shape of the magnetic configuration varies depending on the studied field line while it was shown to be identical over all the field lines (within a flux surface) in quasisymmetric stellarators.

This work inscribes in the development of new strategies for stellarator optimization, e.g. by providing a basis on which to rely for constraining the parameter space of stellarators to be explored.
5. Conclusions
### Chapter 6

**Nomenclature**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>$n$</td>
<td>ion density</td>
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<td>$\tau_E$</td>
<td>energy confinement time</td>
</tr>
<tr>
<td>$T$</td>
<td>ion temperature</td>
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<tr>
<td>$(\psi, \theta, \zeta)$</td>
<td>Boozer coordinates</td>
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<td>$(\psi, \alpha, l)$</td>
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<td>position vector</td>
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<td>i-th covariant basis vector</td>
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<tr>
<td>$\vec{e}^i$</td>
<td>i-th contravariant basis vector</td>
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<td>$\Psi'_t$</td>
<td>derivative with respect to $\psi$ of the toroidal magnetic flux over $2 \pi$</td>
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<td>Jacobian</td>
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<td>$\iota$</td>
<td>rotational transform</td>
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<td>ion mass</td>
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<tr>
<td>$\lambda$</td>
<td>pitch angle of the magnetic field</td>
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Bibliography

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Declaration in lieu of oath

Herewith I declare in lieu of oath that I have prepared this thesis exclusively with the help of my scientific teachers and the means quoted by them.

Madrid, Spain, the 8th of July 2019

Neil Lamas

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