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RELATIVISTIC GUIDING CENTRE DRIFT ORBITS IN CANONICAL AND MAGNETIC COORDINATES

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Relativistic guiding centre drift orbits in canonical and magnetic coordinates

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Abstract

The Hamiltonian formulation of the guiding centre drift orbits for three-dimensional (3D) toroidal configurations with general time dependent electric and magnetic field structures has been extended to cover relativistic particles. For static 3D magnetic fields with nested magnetic surfaces, a mapping procedure from the equilibrium to the canonical coordinates is outlined. This transformation is shown to be so complicated that it renders impractical most applications in canonical coordinates. For magnetic coordinates, the transformation is straightforward. The relativistic guiding centre drift equations are explicitly derived with a constrained perturbed magnetic field that allows these coordinates to adopt a canonical structure.

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1. Introduction

The evaluation of the confinement of α particles in fusion reactor configurations, the application of spectral, particle and other methods to investigate microinstabilities in plasmas and the determination of diffusion coefficients of thermal particles require following individual particle orbits over long time scales. For gyroradii that are small compared with the characteristic spatial dimensions of a magnetic confinement system and for cyclotron frequencies that are large compared with typical frequencies of oscillations of the fields, it is more efficient and effective to follow the guiding centres rather than the exact particle orbits [1,2].

Previous research covering the subject has rather conclusively demonstrated that a Hamiltonian formalism of the guiding centre drift orbits in a coordinate system that displays canonical properties constitutes the most transparent and compact approach for the investigation of this problem [3-12]. The bulk of this work has concentrated on the application of magnetic coordinates introduced by Boozer [13]. These coordinates possess canonical structure when the time dependent perturbed magnetic field is constrained to have a specific representation [3].

The relativistic guiding centre drift orbit problem has been investigated by several authors [4,6,12,14]. Northrop [14] has considered the relativistic drifts directly from the equations of motion rather than from a Hamiltonian perspective. Littlejohn has applied a Hamiltonian formulation first in noncanonical spatial coordinates [4] and subsequently outlined a scheme to obtain the relativistic drifts in Boozer magnetic coordinates [6]. Boozer has considered this problem in further detail [12] using the coordinates that he introduced [13] which retain a canonical structure when a constrained class of perturbed time dependent magnetic fields of the form $\delta\boldsymbol{B} = \boldsymbol{\nabla}\times(\Upsilon\boldsymbol{B})$ is used in toroidal plasmas [3] and has examined applications in magnetospheric plasmas with vanishing toroidal magnetic flux. Meiss and Hazeltine have described a procedure to define canonical coordinates that is valid for arbitrary time dependent electric and magnetic fields [8] and applied it to the nonrelativistic case. We extend their formulation to relativistic guiding centre drifts in this paper and derive the equations of motion. We demonstrate, however, that these general canonical coordinates are rather impractical. The equations of motion that describe the relativistic guiding centre drift orbits are then explicitly obtained in the Boozer magnetic coordinate system (with a restricted representation of the perturbed magnetic field) following the procedure indicated in [12] and carried out for the nonrelativistic case in [5].

The article is organised as follows. In section 2, we extend the Meiss and Hazeltine formulation of the guiding centre drift orbits to relativistic particles in generalised fields adopting the canonical coordinates they introduced. We consider the case of static three dimensional (3D) magnetic fields with nested surfaces in section 3 and describe the mapping to straight field line coordinates in section 4. The transformation from the equilibrium coordinates to the canonical coordinates is investigated in section 5 for arbitrary aspect ratio. The cumbersome nature associated with the mapping to canonical coordinates in general geometry suggests that the magnetic coordinates, despite the constraints imposed on the magnetic field, may be more practical for useful applications. The relativistic drift Hamiltonian presented in [6,12] is thus applied in section 6 to derive the equations of motion that describe the guiding centre drifts in Boozer coordinates. A direct determination of these drifts and convenient initial conditions to follow the trajectories are also discussed. We conclude with a summary in section 7. These relativistic formulations can treat runaway electron phenomena in toroidal plasmas and astrophysical/geomagnetic plasmas.

2. Relativistic guiding centre drifts in canonical coordinates

The canonical momenta in the drift approximation are given by [12]

$$\boldsymbol{P} = p_{\|}\boldsymbol{b} + e\boldsymbol{A} \ , \tag{1}$$

where $\boldsymbol{b}$ is the unit vector along the magnetic field lines, $\boldsymbol{A}$ is the vector potential and e is the the electronic charge of a particle. The corresponding relativistic Hamiltonian is [6,12]

$$\begin{aligned} H = H(\boldsymbol{p}, \boldsymbol{x}, t) &= \sqrt{p_{\|}^2 c^2 + 2\mu B m_0 c^2 + m_0^2 c^4} + e\chi(\boldsymbol{x}, t) \\ &= \gamma m_0 c^2 + e\chi(\boldsymbol{x}, t) \ , \end{aligned} \tag{2}$$

where μ is the magnetic moment, B is the magnitude of the magnetic field, χ is the electrostatic potential, m_0 is the rest mass of the particle, c is the speed of light and γ is the relativistic gamma factor.

As pointed out by Meiss and Hazeltine [8], the basic trick to define canonical coordinates in a toroidal domain with time dependent electric and magnetic fields that can be chaotic is to choose a coordinate system (r, θ, ζ), where r is a radial variable, θ is a poloidal angle and ζ is a toroidal angle, such that the vector potential and the magnetic field in the covariant representation have vanishing radial components, that is

$$\boldsymbol{A} = A_\theta(r, \theta, \zeta, t)\boldsymbol{\nabla}\theta + A_\zeta(r, \theta, \zeta, t)\boldsymbol{\nabla}\zeta \, , \tag{3}$$

$$\boldsymbol{B} = B_\theta(r, \theta, \zeta, t)\boldsymbol{\nabla}\theta + B_\zeta(r, \theta, \zeta, t)\boldsymbol{\nabla}\zeta \, . \tag{4}$$

Considering that $\boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A}$, we can thus write the magnetic field in the contravariant representation as

$$\boldsymbol{B} = \boldsymbol{\nabla}\zeta\times\boldsymbol{\nabla}\psi + \boldsymbol{\nabla}\Phi\times\boldsymbol{\nabla}\theta \, . \tag{5}$$

The poloidal flux function $\psi = -A_\zeta(r, \theta, \zeta, t)$ and the toroidal flux function $\Phi = A_\theta(r, \theta, \zeta, t)$ are arbitrary functions of the spatial coordinates and of time which therefore can cause the magnetic field lines to become chaotic. Consequently, we can express the canonical momenta in the covariant representation as

$$P_\theta = e[\rho_{||} B_\theta(r, \theta, \zeta, t) + \Phi(r, \theta, \zeta, t)] \tag{6}$$

and

$$P_\zeta = e[\rho_{||} B_\zeta(r, \theta, \zeta, t) - \psi(r, \theta, \zeta, t)] \, , \tag{7}$$

respectively. We have defined the parallel gyroradius as $\rho_{||} = p_{||}/(eB)$. We can formally invert these relations to obtain $r = r(P_\theta, P_\zeta, \theta, \zeta, t)$ and $\rho_{||} = \rho_{||}(P_\theta, P_\zeta, \theta, \zeta, t)$, with the angles θ and ζ constituting the spatial canonical coordinates [8]. To realise this, we calculate the derivatives of the canonical momenta with respect to each other which yields a system of linear equations that we can invert to obtain [5]

$$\left.\frac{\partial r}{\partial P_\theta}\right|_{P_\zeta, \theta, \zeta, t} = \frac{B_\zeta}{eD} \, , \tag{8}$$

$$\left.\frac{\partial r}{\partial P_\zeta}\right|_{P_\theta,\theta,\zeta,t} = -\frac{B_\theta}{eD}\,, \tag{9}$$

$$\left.\frac{\partial \rho_\parallel}{\partial P_\theta}\right|_{P_\zeta,\theta,\zeta,t} = \frac{1}{eD}\left(\frac{\partial \psi}{\partial r} - \rho_\parallel \frac{\partial B_\zeta}{\partial r}\right), \tag{10}$$

$$\left.\frac{\partial \rho_\parallel}{\partial P_\zeta}\right|_{P_\theta,\theta,\zeta,t} = \frac{1}{eD}\left(\frac{\partial \Phi}{\partial r} + \rho_\parallel \frac{\partial B_\theta}{\partial r}\right), \tag{11}$$

where the subscripts on the partial derivatives on the left hand side denote what quantities are kept constant. The denominator D is

$$D = B_\zeta \frac{\partial \Phi}{\partial r} + B_\theta \frac{\partial \psi}{\partial r} + \rho_\parallel \left(B_\zeta \frac{\partial B_\theta}{\partial r} - B_\theta \frac{\partial B_\zeta}{\partial r}\right). \tag{12}$$

The equations of motion in the drift approximation are obtained through the evaluation of [5]

$$\dot{P}_\theta = -\left.\frac{\partial H}{\partial \theta}\right|_{P_\theta,P_\zeta,\zeta,t}, \tag{13}$$

$$\dot{P}_\zeta = -\left.\frac{\partial H}{\partial \zeta}\right|_{P_\theta,P_\zeta,\theta,t}, \tag{14}$$

$$\dot{\theta} = \left.\frac{\partial H}{\partial P_\theta}\right|_{P_\zeta,\theta,\zeta,t}, \tag{15}$$

$$\dot{\zeta} = \left.\frac{\partial H}{\partial P_\zeta}\right|_{P_\theta,\theta,\zeta,t}. \tag{16}$$

The evolution equations for the canonical momenta are derived in the Appendix. Using equations (8)-(11), the equations of motion for the canonical angular variables are

$$\dot{\theta} = \frac{eB^2\rho_\parallel}{\gamma m_0 D}\left(\left.\frac{\partial \psi}{\partial r}\right|_{\theta,\zeta,t} - \rho_\parallel \left.\frac{\partial B_\zeta}{\partial r}\right|_{\theta,\zeta,t}\right) + \frac{B_\zeta}{D}\left[\left.\frac{\partial \chi}{\partial r}\right|_{\theta,\zeta,t} + \frac{1}{\gamma}\left(\frac{\mu}{e} + \frac{eB}{m_0}\rho_\parallel^2\right)\left.\frac{\partial B}{\partial r}\right|_{\theta,\zeta,t}\right], \tag{17}$$

$$\dot{\zeta} = \frac{eB^2\rho_\parallel}{\gamma m_0 D}\left(\left.\frac{\partial \Phi}{\partial r}\right|_{\theta,\zeta,t} + \rho_\parallel \left.\frac{\partial B_\theta}{\partial r}\right|_{\theta,\zeta,t}\right) - \frac{B_\theta}{D}\left[\left.\frac{\partial \chi}{\partial r}\right|_{\theta,\zeta,t} + \frac{1}{\gamma}\left(\frac{\mu}{e} + \frac{eB}{m_0}\rho_\parallel^2\right)\left.\frac{\partial B}{\partial r}\right|_{\theta,\zeta,t}\right]. \tag{18}$$

These two relations together with the expressions $\dot{P}_\theta$ and $\dot{P}_\zeta$ shown in the Appendix form the basis of the guiding centre motion in the drift approximation in canonical coordinates. In practical applications, however, it is more convenient to follow the evolution of the radial variable and the parallel gyroradius instead of the canonical momenta. Therefore, we expand

$$\dot{r} = \frac{\partial r}{\partial t} + \left.\frac{\partial r}{\partial P_\theta}\right|_{P_\zeta,\theta,\zeta,t}\dot{P}_\theta + \left.\frac{\partial r}{\partial P_\zeta}\right|_{P_\theta,\theta,\zeta,t}\dot{P}_\zeta + \left.\frac{\partial r}{\partial \theta}\right|_{P_\theta,P_\zeta,\zeta,t}\dot{\theta} + \left.\frac{\partial r}{\partial \zeta}\right|_{P_\theta,P_\zeta,\theta,t}\dot{\zeta}\,, \tag{19}$$

and

$$\dot{\rho_\parallel} = \frac{\partial \rho_\parallel}{\partial t} + \frac{\partial \rho_\parallel}{\partial P_\theta}\bigg|_{P_\zeta,\theta,\zeta,t} \dot{P_\theta} + \frac{\partial \rho_\parallel}{\partial P_\zeta}\bigg|_{P_\theta,\theta,\zeta,t} \dot{P_\zeta} + \frac{\partial \rho_\parallel}{\partial \theta}\bigg|_{P_\theta,P_\zeta,\zeta,t} \dot{\theta} + \frac{\partial \rho_\parallel}{\partial \zeta}\bigg|_{P_\theta,P_\zeta,\theta,t} \dot{\zeta} \,, \tag{20}$$

so after substitution, these forms reduce to

$$\begin{aligned} \dot{r} = \frac{\partial r}{\partial t} &- \frac{B_\zeta}{D}\left[\frac{\partial \chi}{\partial \theta}\bigg|_{r,\zeta,t} + \frac{1}{\gamma}\left(\frac{\mu}{e} + \frac{eB}{m_0}\rho_\parallel^2\right)\frac{\partial B}{\partial \theta}\bigg|_{r,\zeta,t}\right] + \frac{B_\theta}{D}\left[\frac{\partial \chi}{\partial \zeta}\bigg|_{r,\theta,t} + \frac{1}{\gamma}\left(\frac{\mu}{e} + \frac{eB}{m_0}\rho_\parallel^2\right)\frac{\partial B}{\partial \zeta}\bigg|_{r,\theta,t}\right] \\ &- \frac{eB^2\rho_\parallel}{\gamma m_0 D}\left(\frac{\partial \psi}{\partial \theta}\bigg|_{r,\zeta,t} - \rho_\parallel \frac{\partial B_\zeta}{\partial \theta}\bigg|_{r,\zeta,t} + \frac{\partial \Phi}{\partial \zeta}\bigg|_{r,\theta,t} + \rho_\parallel \frac{\partial B_\theta}{\partial \zeta}\bigg|_{r,\theta,t}\right) , \end{aligned} \tag{21}$$

and

$$\begin{aligned} \dot{\rho_\parallel} = \frac{\partial \rho_\parallel}{\partial t} &- \frac{1}{D}\left(\frac{\partial \psi}{\partial r}\bigg|_{\theta,\zeta,t} - \rho_\parallel \frac{\partial B_\zeta}{\partial r}\bigg|_{\theta,\zeta,t}\right)\left[\frac{\partial \chi}{\partial \theta}\bigg|_{r,\zeta,t} + \frac{1}{\gamma}\left(\frac{\mu}{e} + \frac{eB}{m_0}\rho_\parallel^2\right)\frac{\partial B}{\partial \theta}\bigg|_{r,\zeta,t}\right] \\ &- \frac{1}{D}\left(\frac{\partial \Phi}{\partial r}\bigg|_{\theta,\zeta,t} + \rho_\parallel \frac{\partial B_\theta}{\partial r}\bigg|_{\theta,\zeta,t}\right)\left[\frac{\partial \chi}{\partial \zeta}\bigg|_{r,\theta,t} + \frac{1}{\gamma}\left(\frac{\mu}{e} + \frac{eB}{m_0}\rho_\parallel^2\right)\frac{\partial B}{\partial \zeta}\bigg|_{r,\theta,t}\right] \\ &+ \frac{1}{D}\left(\frac{\partial \psi}{\partial \theta}\bigg|_{r,\zeta,t} - \rho_\parallel \frac{\partial B_\zeta}{\partial \theta}\bigg|_{r,\zeta,t}\right)\left[\frac{\partial \chi}{\partial r}\bigg|_{\theta,\zeta,t} + \frac{1}{\gamma}\left(\frac{\mu}{e} + \frac{eB}{m_0}\rho_\parallel^2\right)\frac{\partial B}{\partial r}\bigg|_{\theta,\zeta,t}\right] \\ &+ \frac{1}{D}\left(\frac{\partial \Phi}{\partial \zeta}\bigg|_{r,\theta,t} + \rho_\parallel \frac{\partial B_\theta}{\partial \zeta}\bigg|_{r,\theta,t}\right)\left[\frac{\partial \chi}{\partial r}\bigg|_{\theta,\zeta,t} + \frac{1}{\gamma}\left(\frac{\mu}{e} + \frac{eB}{m_0}\rho_\parallel^2\right)\frac{\partial B}{\partial r}\bigg|_{\theta,\zeta,t}\right] , \end{aligned} \tag{22}$$

respectively. In contrast with the relations for the evolution of the canonical momenta [equations (56) and (57) in the Appendix], the coefficients that multiply the derivatives of r with respect to the canonical angles vanish exactly in the corresponding expressions for $\dot{r}$ and $\dot{\rho_\parallel}$ [equations (21) and (22)]. This is one important reason that makes following $\dot{r}$ and $\dot{\rho_\parallel}$ more useful and effective than $\dot{P_\theta}$ and $\dot{P_\zeta}$. Therefore, equations (17), (18), (21) and (22) constitute the set that govern the relativistic guiding centre motion in the drift approximation.

3. Time independent magnetic fields with nested surfaces

$3D$ magnetic fields with nested magnetic flux surfaces satisfy the condition $\boldsymbol{B} \cdot \boldsymbol{\nabla} s = 0$, where $0 \leq s \leq 1$ is a radial variable that labels the surfaces. This condition and Maxwell's equation $\boldsymbol{\nabla} \cdot \boldsymbol{B} = 0$ imply that the magnetic field can be written in the Clebsch form

$$\boldsymbol{B} = \boldsymbol{\nabla}\alpha \times \boldsymbol{\nabla}\psi \,, \tag{23}$$

where $2\pi\psi(s)$ is the poloidal flux excluded from the surface and α is the field line label given by

$$\alpha = \zeta - q(s)[\theta + \lambda(s,\theta,\zeta)] \,, \tag{24}$$

where θ and ζ are the poloidal and toroidal angular variables, λ is a periodic function of the angles and $q(s) = d\Phi/d\psi$ is the inverse rotational transform. In $3D$ equilibrium configurations with nested magnetic flux surfaces, the force balance relation $\boldsymbol{\nabla} p = \boldsymbol{j} \times \boldsymbol{B}$ with $p = p(s)$ implies that $\boldsymbol{j} \cdot \boldsymbol{\nabla} s = 0$ (the current lines lie on flux surfaces). Furthermore, charge conservation ($\boldsymbol{\nabla} \cdot \boldsymbol{j} = 0$) and Ampère's Law $\mu_0 \boldsymbol{j} = \boldsymbol{\nabla} \times \boldsymbol{B}$ can be combined to express the magnetic field as

$$\boldsymbol{B} = \boldsymbol{\nabla}\eta + \beta\boldsymbol{\nabla} s \,, \tag{25}$$

where

$$\eta = \mu_0[J(s)\theta - I(s)\zeta + Q(s,\theta,\zeta)] \,, \tag{26}$$

$$\beta = \mu_0[I'(s)\zeta - J'(s)\theta - \nu(s,\theta,\zeta)] \,, \tag{27}$$

where $2\pi I(s)$ and $2\pi J(s)$ are the poloidal and toroidal current fluxes, respectively, $Q(s,\theta,\zeta)$ and $\nu(s,\theta,\zeta)$ are periodic functions of θ and ζ, the symbol prime ($'$) denotes the derivative of a flux surface quantity with respect to s and the permeability of free space is μ_0.

4. The mapping procedure to straight field line coordinates

Suppose an equilibrium state is known in some arbitrary coordinate system (s,u,v), typically for example that used in the VMEC code [15]. In the transformation, we retain the radial variable that identifies the flux contours but allow the angular variables to change. Thus we define the transformation

$$\theta = u + h(s,u,v) \,, \tag{28}$$

$$\zeta = v + k(s,u,v) \,, \tag{29}$$

where h and k are periodic functions of the angles poloidal and toroidal angles u and v, respectively. A coordinate system with straight magnetic field lines satisfies the condition

$$\lambda(s,\theta,\zeta) = 0 \,. \tag{30}$$

The functions α, η and β, being scalars, are invariant with respect to coordinate transformations. Substituting the forms of θ and ζ into the expressions for α and η given by equations (24) and (26), respectively, we obtain

$$h(s,u,v) = \frac{Q_v(s,u,v) - Q(s,\theta,\zeta) - q(s)I(s)\lambda(s,u,v)}{J(s) - q(s)I(s)} \,, \tag{31}$$

$$k(s,u,v) = q(s)\frac{Q_v(s,u,v) - Q(s,\theta,\zeta) - J(s)\lambda(s,u,v)}{J(s) - q(s)I(s)} \,. \tag{32}$$

Here the function $Q(s,\theta,\zeta) = Q[s,\theta(s,u,v),\zeta(s,u,v)]$ must still be specified. Typical examples are the magnetic coordinates introduced by Boozer [13] where $Q = Q_b(s,\theta_b,\zeta_b) = 0$, the PEST-1 coordinates where the toroidal angle is invariant [16] yielding $h(s,u,v) = \lambda(s,u,v)$ which entails $Q_p = Q_v - J(s)\lambda(s,u,v)$ or that where the poloidal angle is fixed and the toroidal angle is modified to straighten the field lines, $Q_d = Q_v - q(s)I(s)\lambda(s,u,v)$ which implies $k(s,u,v) = -q(s)\lambda(s,u,v)$ [17]. Other straight field line coordinates of interest have been proposed that specify the Jacobian as some prescribed function, namely

$$\nabla\theta\times\nabla\zeta\cdot\nabla s = \frac{1}{\sqrt{g}(s,u,v)} \,. \tag{33}$$

The Hamada coordinates [15]constitute the best known example for which the Jacobian is unity. Substituting θ and ζ in (33) using equations (28) and (29), we have the relation

$$\frac{\partial h}{\partial u} + \frac{\partial k}{\partial v} + \frac{\partial h}{\partial u}\frac{\partial k}{\partial v} - \frac{\partial h}{\partial v}\frac{\partial k}{\partial u} = \frac{1}{\sqrt{g}(s,u,v)} - 1 \,. \tag{34}$$

The nonlinearity in this equation is only apparent as combining it with the expressions for h and k given in equations (31) and (32), we obtain

$$\left[1 - q(s)\frac{\partial\lambda}{\partial v}\right]\frac{\partial h}{\partial u} + q(s)\left(1 + \frac{\partial\lambda}{\partial u}\right)\frac{\partial h}{\partial v} = \frac{1}{\sqrt{g}(s,u,v)} - 1 + q(s)\frac{\partial\lambda}{\partial v} \,. \tag{35}$$

This constitutes a magnetic differential equation as the operator on the left hand side can be readily identified as $\sqrt{g}\boldsymbol{B}\cdot\nabla/\psi'(s)$. Therefore, all coordinate transformations that rely on the specification of the Jacobian in 3D systems with nested magnetic surfaces are singular on mode rational surfaces. This has already been specifically pointed out for Hamada coordinates [18].

5. The mapping to canonical coordinates

For time independent toroidal 3D magnetic fields with nested surfaces, the field lines in canonical coordinates are straight [8]. Labelling the canonical coordinates as (s,θ_c,ζ_c), the function $Q = Q_c(s,\theta_c,\zeta_c)$ is unknown. To solve for it, we must invoke the expression for β [equation (27)] to get

$$\nu_c[s,\theta_c(s,u,v),\zeta_c(s,u,v)] = \nu_v(s,u,v) + J'(s)h(s,u,v) - I'(s)k(s,u,v) \ , \tag{36}$$

and combine it with the condition that the radial magnetic field component in the covariant representation vanishes for general canonical coordinates, namely

$$B_s = -\mu_0\Big[\nu_c(s,\theta_c,\zeta_c) + \frac{\partial Q_c}{\partial s}\Big|_{\theta_c,\zeta_c}\Big] = 0 \ . \tag{37}$$

to obtain

$$\begin{aligned}\frac{\partial Q_c}{\partial s}\Big|_{\theta_c,\zeta_c} + \frac{J'(s)-q(s)I'(s)}{J(s)-q(s)I(s)}Q_c = \nu_v(s,u,v) + \frac{J'(s)-q(s)I'(s)}{J(s)-q(s)I(s)}Q_v(s,u,v) \\ + q(s)\frac{I'(s)J(s)-J'(s)I(s)}{J(s)-q(s)I(s)}\lambda(s,u,v) \ .\end{aligned} \tag{38}$$

The derivative of Q_c with respect to s is evaluated at fixed θ_c and ζ_c. Therefore, invoking the transformation functions, we can write

$$\begin{aligned}\frac{\partial Q_c}{\partial s}\Big|_{\theta_c,\zeta_c} = \frac{\partial Q_c}{\partial s}\Big|_{u,v} &+ \frac{\left[\frac{\partial h}{\partial v}\frac{\partial k}{\partial s} - \frac{\partial h}{\partial s}\left(1+\frac{\partial k}{\partial v}\right)\right]}{\left[\left((1+\frac{\partial h}{\partial u}\right)\left(1+\frac{\partial k}{\partial v}\right) - \frac{\partial h}{\partial v}\frac{\partial k}{\partial u}\right]}\frac{\partial Q_c}{\partial u}\Big|_{v,s} \\ &+ \frac{\left[\frac{\partial h}{\partial s}\frac{\partial k}{\partial u} - \frac{\partial k}{\partial s}\left(1+\frac{\partial h}{\partial u}\right)\right]}{\left[\left((1+\frac{\partial h}{\partial u}\right)\left(1+\frac{\partial k}{\partial v}\right) - \frac{\partial h}{\partial v}\frac{\partial k}{\partial u}\right]}\frac{\partial Q_c}{\partial v}\Big|_{s,u} \ .\end{aligned} \tag{39}$$

Performing a Fourier transformation leads a very complicated set of nonlinear ordinary differential equations. Thus, we conclude that the canonical coordinates, though allowing a very elegant and concise formulation of the guiding centre drift orbits, are impractical for most fundamental applications because the transformation to these coordinates is so cumbersome to realise.

6. Relativistic guiding centre drifts in magnetic coordinates

The Boozer magnetic coordinates [13] are applicable to 3D plasma confinement systems in which the unperturbed magnetic field forms perfect toroidal surfaces. Then $\psi = \psi(s)$ and $\Phi = \Phi(s)$. We shall label these coordinates in this section with (s,ϑ,ϕ), where the Boozer angle ϑ is different and should not be confused with the canonical poloidal angle θ defined in section 2. The specification of this coordinate system, however, allows the introduction of a magnetic field perturbation of the form

$$\delta \boldsymbol{B} = \boldsymbol{\nabla}\times[\Upsilon(s,\vartheta,\phi,t)\boldsymbol{B}]\,, \tag{40}$$

which can cause ergodic behaviour, but is not completely general in nature [3,5]. Nevertheless, it is adequate to accurately describe the radial component of any perturbed magnetic field. The other components only introduce nonresonant contributions and thus are less important. This approximation allows the magnetic coordinates to constitute canonical coordinates. The unperturbed magnetic field in the contravariant representation is given by equations (23) and (24) with $\lambda = 0$ and in the covariant representation by equations (25)-(27) with $Q = 0$. The vector potential in the Boozer coordinates is

$$\boldsymbol{A} = \Phi(s)\boldsymbol{\nabla}\vartheta - \psi(s)\boldsymbol{\nabla}\phi + \Upsilon(s,\vartheta,\phi,t)\boldsymbol{B}\,. \tag{41}$$

To first order in gyroradius, the canonical momenta are $P_\vartheta = e[\Phi(s) + \rho_c\mu_0 J(s)]$ and $P_\phi = -e[\psi(s) + \rho_c\mu_0 I(s)]$ where the effective gyroradius [5] valid for a relativistic particle is $\rho_c = p_{||}/(eB) + \Upsilon$. From these relations we see that $s = s(P_\vartheta, P_\phi)$ and $\rho_c = \rho_c(P_\vartheta, P_\phi)$. Following the same procedure outlined in section 2, we derive the derivatives of s and ρ_c with respect to the canonical momenta. These correspond to equations (8)-(11) with s replacing r and ρ_c replacing $\rho_{||}$, respectively. The denominator D acquires the form

$$D = D_b = \mu_0[\psi'(s)J(s) - \Phi'(s)I(s)]\left[1 + \mu_0\rho_c\frac{J(s)I'(s) - I(s)J'(s)}{\psi'(s)J(s) - \Phi'(s)I(s)}\right]\,. \tag{42}$$

The equations of motion described in (13)-(16) can be straightforwardly analysed to obtain

$$\dot{P}_\vartheta = -\,e\left[\frac{\partial\chi}{\partial\vartheta}\bigg|_{s,\phi,t} + \frac{1}{\gamma}\left(\frac{\mu}{e} + \frac{eB}{m_0}\rho_{||}^2\right)\frac{\partial B}{\partial\vartheta}\bigg|_{s,\phi} - \frac{eB^2\rho_{||}}{\gamma m_0}\frac{\partial\Upsilon}{\partial\vartheta}\bigg|_{s,\phi,t}\right]\,, \tag{43}$$

$$\dot{P}_\phi = -\,e\left[\frac{\partial\chi}{\partial\phi}\bigg|_{s,\vartheta,t} + \frac{1}{\gamma}\left(\frac{\mu}{e} + \frac{eB}{m_0}\rho_{||}^2\right)\frac{\partial B}{\partial\phi}\bigg|_{s,\vartheta} - \frac{eB^2\rho_{||}}{\gamma m_0}\frac{\partial\Upsilon}{\partial\phi}\bigg|_{s,\vartheta,t}\right]\,, \tag{44}$$

$$\begin{aligned}\dot{\vartheta} = &-\frac{eB^2\rho_{||}}{\gamma m_0 D_b}\left[\psi'(s) + (\rho_{||} + \Upsilon)\mu_0 I'(s) + \mu_0 I(s)\frac{\partial\Upsilon}{\partial s}\bigg|_{\vartheta,\phi,t}\right] \\ &-\frac{\mu_0 I(s)}{D_b}\left[\frac{\partial\chi}{\partial s}\bigg|_{\vartheta,\phi,t} + \frac{1}{\gamma}\left(\frac{\mu}{e} + \frac{eB}{m_0}\rho_{||}^2\right)\frac{\partial B}{\partial s}\bigg|_{\vartheta,\phi}\right]\,,\end{aligned} \tag{45}$$

$$\begin{aligned}\dot{\phi} = &-\frac{eB^2\rho_{||}}{\gamma m_0 D_b}\left[\Phi'(s) + (\rho_{||} + \Upsilon)\mu_0 J'(s) + \mu_0 J(s)\frac{\partial\Upsilon}{\partial s}\bigg|_{\vartheta,\phi,t}\right] \\ &-\frac{\mu_0 J(s)}{D_b}\left[\frac{\partial\chi}{\partial s}\bigg|_{\vartheta,\phi,t} + \frac{1}{\gamma}\left(\frac{\mu}{e} + \frac{eB}{m_0}\rho_{||}^2\right)\frac{\partial B}{\partial s}\bigg|_{\vartheta,\phi}\right]\,,\end{aligned} \tag{46}$$

respectively. Rather than follow the evolution of the canonical momenta, it is more convenient to evaluate $\dot{s}$ and $\dot{\rho}_{\|}$, namely

$$\dot{s} = \frac{\partial s}{\partial P_\vartheta}\bigg|_{P_\phi,\vartheta,\phi,t} \dot{P}_\vartheta + \frac{\partial s}{\partial P_\phi}\bigg|_{P_\vartheta,\vartheta,\phi,t} \dot{P}_\phi \,, \tag{47}$$

and with $\rho_{\|} = \rho_c - \Upsilon$,

$$\begin{aligned}\dot{\rho}_{\|} &= \dot{\rho}_c - \frac{d\Upsilon}{dt} \\ &= \frac{\partial \rho_c}{\partial P_\vartheta}\bigg|_{P_\phi,\vartheta,\phi,t} \dot{P}_\vartheta + \frac{\partial \rho_c}{\partial P_\phi}\bigg|_{P_\vartheta,\vartheta,\phi,t} \dot{P}_\phi - \frac{\partial \Upsilon}{\partial s}\bigg|_{\vartheta,\phi,t} \dot{s} - \frac{\partial \Upsilon}{\partial \vartheta}\bigg|_{s,\phi,t} \dot{\vartheta} - \frac{\partial \Upsilon}{\partial \phi}\bigg|_{s,\vartheta,t} \dot{\phi} - \frac{\partial \Upsilon}{\partial t}\bigg|_{s,\vartheta,\phi} ,\end{aligned} \tag{48}$$

from which we obtain

$$\begin{aligned}\dot{s} = \; & \frac{\mu_0 I(s)}{D_b}\left[\frac{\partial \chi}{\partial \vartheta}\bigg|_{s,\phi,t} + \frac{1}{\gamma}\left(\frac{\mu}{e} + \frac{eB}{m_0}\rho_{\|}^2\right)\frac{\partial B}{\partial \vartheta}\bigg|_{s,\phi} - \frac{eB^2\rho_{\|}}{\gamma m_0}\frac{\partial \Upsilon}{\partial \vartheta}\bigg|_{s,\phi,t}\right] \\ & + \frac{\mu_0 J(s)}{D_b}\left[\frac{\partial \chi}{\partial \phi}\bigg|_{s,\vartheta,t} + \frac{1}{\gamma}\left(\frac{\mu}{e} + \frac{eB}{m_0}\rho_{\|}^2\right)\frac{\partial B}{\partial \phi}\bigg|_{s,\vartheta} - \frac{eB^2\rho_{\|}}{\gamma m_0}\frac{\partial \Upsilon}{\partial \phi}\bigg|_{s,\vartheta,t}\right] ,\end{aligned} \tag{49}$$

and

$$\begin{aligned}\dot{\rho}_{\|} = & - \frac{1}{D_b}\left[\psi'(s) + (\rho_{\|} + \Upsilon)\mu_0 I'(s) + \mu_0 I(s)\frac{\partial \Upsilon}{\partial s}\bigg|_{\vartheta,\phi,t}\right]\left[\frac{\partial \chi}{\partial \vartheta}\bigg|_{s,\phi,t} + \frac{1}{\gamma}\left(\frac{\mu}{e} + \frac{eB}{m_0}\rho_{\|}^2\right)\frac{\partial B}{\partial \vartheta}\bigg|_{s,\phi}\right] \\ & - \frac{1}{D_b}\left[\Phi'(s) + (\rho_{\|} + \Upsilon)\mu_0 J'(s) + \mu_0 J(s)\frac{\partial \Upsilon}{\partial s}\bigg|_{\vartheta,\phi,t}\right]\left[\frac{\partial \chi}{\partial \phi}\bigg|_{s,\vartheta,t} + \frac{1}{\gamma}\left(\frac{\mu}{e} + \frac{eB}{m_0}\rho_{\|}^2\right)\frac{\partial B}{\partial \phi}\bigg|_{s,\vartheta}\right] \\ & - \frac{\mu_0}{D_b}\left[I(s)\frac{\partial \Upsilon}{\partial \vartheta}\bigg|_{s,\phi,t} + J(s)\frac{\partial \Upsilon}{\partial \phi}\bigg|_{s,\vartheta,t}\right]\left[\frac{\partial \chi}{\partial s}\bigg|_{\vartheta,\phi,t} + \frac{1}{\gamma}\left(\frac{\mu}{e} + \frac{eB}{m_0}\rho_{\|}^2\right)\frac{\partial B}{\partial s}\bigg|_{\vartheta,\phi}\right] - \frac{\partial \Upsilon}{\partial t}\bigg|_{s,\vartheta,\phi} ,\end{aligned} \tag{50}$$

respectively. Therefore, the set of equations (45), (46), (49) and (50) constitute the governing system for the guiding centre drift motion in Boozer magnetic coordinates. Their structure is quite similar to those derived in the general canonical coordinates described in section 2. In the nonrelativistic limit, they recover the forms derived by White and Chance [5] when the different normalisation they applied is taken into account.

6.1. Direct determination of the guiding centre drifts

The guiding centre drift velocity expressed in a form that retains the relevant components to second order in the gyroradius [2] that it satisfies Louisville's theorem and conservation laws in symmetric systems [3] valid for relativistic particles can be written as

$$\boldsymbol{v_d} = \frac{e\rho_{\|}}{\gamma m_0[1 + (\rho_{\|} + \Upsilon)\mu_0 \boldsymbol{j}\cdot\boldsymbol{B}/B^2]}\{\boldsymbol{B} + \boldsymbol{\nabla}\times[(\rho_{\|} + \Upsilon)\boldsymbol{B}]\} \,. \tag{51}$$

A direct evaluation of the guiding centre drifts follows from $\dot{s} = \boldsymbol{v_d} \cdot \boldsymbol{\nabla} s$, $\dot{\vartheta} = \boldsymbol{v_d} \cdot \boldsymbol{\nabla}\vartheta$, $\dot{\phi} = \boldsymbol{v_d} \cdot \boldsymbol{\nabla}\phi$ and $\dot{\rho}_{\|} = \boldsymbol{v_d} \cdot \boldsymbol{\nabla}\rho_{\|}$ [20]. The analysis is simplified by noting that $\rho_{\|}=\rho_{\|}(B,\chi)$. Expanding

$$\frac{\mu_0 \boldsymbol{j} \cdot \boldsymbol{B}}{B^2} = \frac{\mu_0[J(s)I'(s) - I(s)J'(s)] + I(s)\frac{\partial B_s}{\partial \vartheta} + J(s)\frac{\partial B_s}{\partial \phi}}{\psi'(s)J(s) - \Phi'(s)I(s)}, \tag{52}$$

we arrive at the conclusion that the resulting expression for $\dot{s}$ recovers equation (49) if we ignore the derivatives of B_s in the numerator of (52), which are formally of higher order as B_s is proportional to the pressure gradient (hence to the ratio of kinetic to magnetic pressures). This constitutes an alternative manner to derive the guiding centre drifts and is helpful to verify the accuracy of the expressions obtained. Similarly, the direct evaluation of $\dot{\vartheta}$, $\dot{\phi}$ and $\dot{\rho}_{\|}$ recover the corresponding relations obtained from the Hamiltonian formulation if the additional higher order terms containing B_s that appear are neglected.

6.2. Initial conditions

In order to follow the guiding centre drift trajectories, it is necessary to provide the positions in real space and two momentum variables as initial conditions. Thus the starting values of the spatial coordinates (s, ϑ, ϕ) for the guiding centre orbit of each particle must be specified. One convenient velocity space variable is the initial relativistic gamma factor γ_i from which the particle energy $\varepsilon_{pi} = \gamma_i m_0 c^2$ is obtained. A second convenient variable to specify is the initial pitch angle given by $p_{\|}/p$ (the ratio of the parallel to the total particle momemtum). The initial particle momentum is related to γ_i through $p_i = \sqrt{(\gamma_i^2 - 1)} m_0 c$, whence we obtain the initial values of $p_{\|}$ and of the gyroradius. The determination of the perpendicular component of the momentum $p_{\perp i}$ follows. This permits us to obtain the magnetic moment $\mu = p_{\perp}^2/(2m_0 B)$ which is a constant of the motion.

7. Summary

We have extended the elegant formulation of the guiding centre drift orbits in the canonical coordinates proposed by Meiss and Hazeltine [8] which can treat trajectories in completely arbitrary time dependent magnetic fields that can even be chaotic to relativistic particles. We have explicitly derived the equations for the evolution of the spatial coordinates and of the parallel gyroradius that govern the guiding centre drift motion. We have considered the case of a 3D equilibrium with nested magnetic flux surfaces and have developed the mapping procedure from the coordinates of the equilibrium state to the general canonical coordinates. We have demonstrated, however, that the equations that describe the transformation to the canonical coordinates are much too complicated for fundamental practical applications.

In contrast, the transformation to Boozer magnetic coordinates are straightforward to implement as outlined in section 4 and previously described also in [19,21]. Thus, we have formulated the guiding centre drift orbits for relativistic particles in magnetic coordinates as well. However, for the magnetic coordinates to have a canonical structure, the perturbed magnetic field must be constrained to have the form $\delta \boldsymbol{B} = \boldsymbol{\nabla} \times (\Upsilon \boldsymbol{B})$ which, nevertheless, adequately captures the essential features of the radial component of any arbitrary field [3,5]. The evolution equations for the spatial coordinates and for the parallel gyroradius are explicitly derived in these coordinates. When the electric and magnetic fields are independent of time, the equation of motion for the parallel gyroradius is redundant because the particle energy becomes a constant of the motion.

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Appendix

The derivatives of the Hamiltonian with respect to the canonical angles require knowing the corresponding derivatives of the parallel gyroradius. These are calculated by examining the derivatives of the canonical momenta with respect to the canonical angles (which by definition vanish). Furthermore, the derivatives of H and $\rho_{||}$ with respect to the canonical angles require the evaluation of the derivatives of B, B_θ, B_ζ, Φ, ψ and χ with respect to θ and ζ at fixed P_θ and P_ζ. However, these quantities are functions of r, θ, ζ and t. We note, however, that for any function $K(r, \theta, \zeta, t)$, we have

$$\left.\frac{\partial K}{\partial \theta}\right|_{P_\theta, P_\zeta, \zeta, t} = \left.\frac{\partial K}{\partial \theta}\right|_{r, \zeta, t} + \left.\frac{\partial K}{\partial r}\right|_{\theta, \zeta, t} \left.\frac{\partial r}{\partial \theta}\right|_{P_\theta, P_\zeta, \zeta, t} . \tag{53}$$

A corresponding relation applies for the derivative with respect to ζ. Then, the derivatives of interest of the parallel gyroradius are

$$\left.\frac{\partial\rho_\parallel}{\partial\theta}\right|_{P_\theta,P_\zeta,\zeta,t} = \frac{1}{B_\zeta}\left[\left.\frac{\partial\psi}{\partial\theta}\right|_{r,\zeta,t} - \rho_\parallel\left.\frac{\partial B_\zeta}{\partial\theta}\right|_{r,\zeta,t} + \left(\left.\frac{\partial\psi}{\partial r}\right|_{\theta,\zeta,t} - \rho_\parallel\left.\frac{\partial B_\zeta}{\partial r}\right|_{\theta,\zeta,t}\right)\left.\frac{\partial r}{\partial\theta}\right|_{P_\theta,P_\zeta,\zeta,t}\right], \tag{54}$$

$$\left.\frac{\partial\rho_\parallel}{\partial\zeta}\right|_{P_\theta,P_\zeta,\theta,t} = -\frac{1}{B_\theta}\left[\left.\frac{\partial\Phi}{\partial\zeta}\right|_{r,\theta,t} + \rho_\parallel\left.\frac{\partial B_\theta}{\partial\zeta}\right|_{r,\theta,t} + \left(\left.\frac{\partial\Phi}{\partial r}\right|_{\theta,\zeta,t} + \rho_\parallel\left.\frac{\partial B_\theta}{\partial r}\right|_{\theta,\zeta,t}\right)\left.\frac{\partial r}{\partial\zeta}\right|_{P_\theta,P_\zeta,\theta,t}\right], \tag{55}$$

respectively. Consequently, the equations of motion for the canonical momenta become

$$\begin{aligned}\dot{P}_\theta = &-e\left[\left.\frac{\partial\chi}{\partial\theta}\right|_{r,\zeta,t} + \frac{1}{\gamma}\left(\frac{\mu}{e} + \frac{eB}{m_0}\rho_\parallel^2\right)\left.\frac{\partial B}{\partial\theta}\right|_{r,\zeta,t} + \frac{eB^2\rho_\parallel}{\gamma m_0 B_\zeta}\left(\left.\frac{\partial\psi}{\partial\theta}\right|_{r,\zeta,t} - \rho_\parallel\left.\frac{\partial B_\zeta}{\partial\theta}\right|_{r,\zeta,t}\right)\right] \\ &-e\left[\left.\frac{\partial\chi}{\partial r}\right|_{\theta,\zeta,t} + \frac{1}{\gamma}\left(\frac{\mu}{e} + \frac{eB}{m_0}\rho_\parallel^2\right)\left.\frac{\partial B}{\partial r}\right|_{\theta,\zeta,t} + \frac{eB^2\rho_\parallel}{\gamma m_0 B_\zeta}\left(\left.\frac{\partial\psi}{\partial r}\right|_{\theta,\zeta,t} - \rho_\parallel\left.\frac{\partial B_\zeta}{\partial r}\right|_{\theta,\zeta,t}\right)\right]\left.\frac{\partial r}{\partial\theta}\right|_{P_\theta,P_\zeta,\zeta,t},\end{aligned} \tag{56}$$

$$\begin{aligned}\dot{P}_\zeta = &-e\left[\left.\frac{\partial\chi}{\partial\zeta}\right|_{r,\theta,t} + \frac{1}{\gamma}\left(\frac{\mu}{e} + \frac{eB}{m_0}\rho_\parallel^2\right)\left.\frac{\partial B}{\partial\zeta}\right|_{r,\theta,t} - \frac{eB^2\rho_\parallel}{\gamma m_0 B_\theta}\left(\left.\frac{\partial\Phi}{\partial\zeta}\right|_{r,\theta,t} + \rho_\parallel\left.\frac{\partial B_\theta}{\partial\zeta}\right|_{r,\theta,t}\right)\right] \\ &-e\left[\left.\frac{\partial\chi}{\partial r}\right|_{\theta,\zeta,t} + \frac{1}{\gamma}\left(\frac{\mu}{e} + \frac{eB}{m_0}\rho_\parallel^2\right)\left.\frac{\partial B}{\partial r}\right|_{\theta,\zeta,t} - \frac{eB^2\rho_\parallel}{\gamma m_0 B_\theta}\left(\left.\frac{\partial\Phi}{\partial r}\right|_{\theta,\zeta,t} + \rho_\parallel\left.\frac{\partial B_\theta}{\partial r}\right|_{\theta,\zeta,t}\right)\right]\left.\frac{\partial r}{\partial\zeta}\right|_{P_\theta,P_\zeta,\theta,t}.\end{aligned} \tag{57}$$

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