Definitions for GS2 full-flux-surface stellarator geometry

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In this note, we state the definitions used for geometric quantities in the full-flux-surface version of GS2, and we detail how these quantities are computed from the information in a VMEC output file. We also derive how the twist-and-shift parallel boundary condition and box size quantization conditions, familiar from flux tube simulations, are modified in a full-surface calculation.

1 Review of GS2 geometry definitions

1.1 Definitions valid for any GS2 geometry

First, we review the definitions used in the flux tube version of GS2, as discussed in the note `gs2_geometry_definitions.pdf`. The Clebsch representation of the magnetic field is

$$\boldsymbol{B} = \nabla\psi \times \nabla\alpha. \tag{1}$$

We take ψ to represent a flux surface label, but do not (yet) assume that it is necessarily the poloidal or toroidal flux. The α coordinate is a field line label on the flux surface. New coordinates $x = x(\psi)$ and $y = y(\alpha)$ are introduced that are scaled versions of ψ and α with dimensions of length. In a flux tube simulation where x and y only vary on a length scale comparable to the gyroradius, then

$$\begin{aligned} x &= \frac{dx}{d\psi}\left[\psi - \psi_0\right], \\ y &= \frac{dy}{d\alpha}\left[\alpha - \alpha_0\right], \end{aligned} \tag{2}$$

where $dx/d\psi$ and $dy/d\alpha$ are constant within the flux tube, and ψ_0 and α_0 are the coordinates around which the flux tube is centered.

A reference magnetic field strength B_{ref} and reference length L_{ref} are introduced for normalization. Then the quantities needed to specify the geometry in GS2 are the following:

$$\texttt{bmag} = \frac{B}{B_{ref}}, \tag{3}$$

$$\texttt{gradpar} = L_{ref}\nabla_{||}z, \tag{4}$$

$$\texttt{gds2} = |\nabla y|^2 = \left(\frac{dy}{d\alpha}\right)^2 |\nabla\alpha|^2, \tag{5}$$

$$\texttt{gds21} = \hat{s}\nabla x \cdot \nabla y = \hat{s}\frac{dx}{d\psi}\frac{dy}{d\alpha}\nabla\psi \cdot \nabla\alpha, \tag{6}$$

$$\texttt{gds22} = \hat{s}^2|\nabla x|^2 = \hat{s}^2\left(\frac{dx}{d\psi}\right)^2 |\nabla\psi|^2. \tag{7}$$

$$\texttt{gbdrift} = \frac{2B_{ref}L_{ref}}{B^3}\boldsymbol{B} \times \nabla B \cdot \nabla y, \tag{8}$$

$$\texttt{gbdrift0} = \hat{s}\frac{2B_{ref}L_{ref}}{B^3}\boldsymbol{B} \times \nabla B \cdot \nabla x, \tag{9}$$

$$\texttt{cvdrift} = \frac{2B_{ref}L_{ref}}{B^2}\boldsymbol{B} \times \boldsymbol{\kappa} \cdot \nabla y, \tag{10}$$

$$\texttt{cvdrift0} = \hat{s}\frac{2B_{ref}L_{ref}}{B^2}\boldsymbol{B} \times \boldsymbol{\kappa} \cdot \nabla x, \tag{11}$$

$$\texttt{kxfac} = B_{ref}\frac{dx}{d\psi}\frac{dy}{d\alpha}, \tag{12}$$

$$\texttt{fprim} = B_{ref}L_{ref}\frac{dy}{d\alpha}\frac{dx}{d\psi}\frac{1}{n_s}\frac{dn_s}{dx}, \tag{13}$$

$$\texttt{tprim} = B_{ref}L_{ref}\frac{dy}{d\alpha}\frac{dx}{d\psi}\frac{1}{T_s}\frac{dT_s}{dx}. \tag{14}$$

These quantities are all dimensionless. In the definition of `gradpar`, z is any parallel coordinate; the parallel coordinate is called `theta` in GS2, although it need not be the poloidal angle. Also $\hat{s}$ is whichever number is used to define θ_0 =`theta0` in the relation

$$\theta_0 = \frac{k_x}{\hat{s}k_y}. \tag{15}$$

The above quantities (3)-(11) are functions of the parallel coordinate z. The quantity `kxfac` is a single number, and the quantities `fprim` and `tprim` are each single numbers for each particle species.

Since $\boldsymbol{B} \times \boldsymbol{\kappa} \cdot \nabla\psi = \boldsymbol{b} \times \nabla B \cdot \nabla\psi$ for any static ideal MHD equilibrium (at any β), then `cvdrift0` = `gbdrift0`.

1.2 Definitions used previously for stellarator geometry in GS2

In stellarator calculations that have been performed using the standard flux tube version of GS2 and the GIST geometry interface, the following additional definitions have been made. The flux surface label ψ has been taken to be the toroidal flux divided by 2π. Therefore for consistency with (1), $\alpha = \theta - \iota\zeta$ where $\iota = 1/q$ is the rotational transform, q is the safety factor, and θ and ζ are straight-field-line poloidal and toroidal angles. While the GIST GS2 interface takes θ and ζ to be Boozer angles, all the expressions below are equally valid for other straight-field-line angles such as PEST or Hamada coordinates.

In GIST, the parallel coordinate z is presently taken to be the Boozer poloidal angle. However none of the expressions in this note are altered if a different choice is desired.

In GIST, the reference length L_{ref} is taken to be the effective minor radius computed by VMEC, named Aminor_p in the VMEC wout*.nc file. The reference magnetic field is taken to be

$$B_{ref} = \frac{2\psi_{LCFS}}{L_{ref}^2} \tag{16}$$

where ψ_{LCFS} is the value of ψ at the outermost VMEC flux surface. The choice (16) is motivated by the cylindrical limit: the toroidal flux enclosed by the outermost VMEC surface is equivalent to the flux of a field B_{ref} through a circle of radius L_{ref}.

The radial coordinate x is then chosen to be

$$x = L_{ref}\sqrt{\frac{\psi}{\psi_{LCFS}}} = L_{ref}\sqrt{s}, \tag{17}$$

where $s = \psi/\psi_{LCFS} \in [0, 1]$ is the flux surface label coordinate used in VMEC. The choice (17) is natural since x then reduces to the usual minor radius in the cylindrical limit. It follows that

$$\frac{dx}{d\psi} = \frac{L_{ref}}{2\sqrt{\psi\psi_{LCFS}}} = \frac{1}{L_{ref}B_{ref}}\sqrt{\frac{\psi_{LCFS}}{\psi}}. \tag{18}$$

Another choice made in GIST is `kxfac` $= 1$. According to (12), we are then required to take

$$\frac{dy}{d\alpha} = L_{ref}\sqrt{\frac{\psi}{\psi_{LCFS}}}. \tag{19}$$

GIST computes the global shear parameter $\hat{s}$ using

$$\hat{s} = \frac{x}{q}\frac{dq}{dx}. \tag{20}$$

Now that $dx/d\psi$ and $dy/d\alpha$ are specified, equations (3)-(14) can be evaluated to obtain explicit expressions for the geometry arrays computed by GIST for GS2:

$$\begin{aligned}
\texttt{bmag} &= B/B_{ref}, &(21)\\
\texttt{gradpar} &= L_{ref}\nabla_{||}z, &(22)\\
\texttt{gds2} &= |\nabla y|^2 = |\nabla\alpha|^2 L_{ref}^2 \frac{\psi}{\psi_{LCFS}}, &(23)\\
\texttt{gds21} &= \hat{s}\nabla x\cdot\nabla y = \frac{\hat{s}}{B_{ref}}\nabla\psi\cdot\nabla\alpha, &(24)\\
\texttt{gds22} &= \hat{s}^2|\nabla x|^2 = \left(\frac{\hat{s}}{L_{ref}B_{ref}}\right)^2 \frac{\psi_{LCFS}}{\psi}|\nabla\psi|^2, &(25)\\
\texttt{gbdrift} &= \frac{2B_{ref}L_{ref}^2}{B^3}\sqrt{\frac{\psi}{\psi_{LCFS}}}\boldsymbol{B}\times\nabla B\cdot\nabla\alpha, &(26)\\
\texttt{gbdrift0} &= \hat{s}\frac{2}{B^3}\sqrt{\frac{\psi_{LCFS}}{\psi}}\boldsymbol{B}\times\nabla B\cdot\nabla\psi, &(27)\\
\texttt{cvdrift} &= \frac{2B_{ref}L_{ref}^2}{B^2}\sqrt{\frac{\psi}{\psi_{LCFS}}}\boldsymbol{B}\times\boldsymbol{\kappa}\cdot\nabla\alpha, &(28)\\
\texttt{cvdrift0} &= \hat{s}\frac{2}{B^2}\sqrt{\frac{\psi_{LCFS}}{\psi}}\boldsymbol{B}\times\boldsymbol{\kappa}\cdot\nabla\psi, &(29)\\
\texttt{fprim} &= \frac{L_{ref}}{n_s}\frac{dn_s}{dx}, &(30)\\
\texttt{tprim} &= \frac{L_{ref}}{T_s}\frac{dT_s}{dx}. &(31)
\end{aligned}$$

2 VMEC coordinates

The VMEC code uses a toroidal coordinate ζ which is the conventional azimuthal angle of cylindrical coordinates.

We let θ_v denote the poloidal angle used in VMEC, which is *not* a straight-field-line coordinate. We also let θ_p denote the PEST poloidal angle, i.e. the straight-field-line angle which results when the toroidal angle is chosen to be the conventional azimuthal angle of cylindrical coordinates, as in VMEC. The conversion between the two coordinates is

$$\theta_p = \theta_v + \Lambda, \tag{32}$$

where Λ is the quantity given by the `lmns` and `lmnc` arrays in VMEC. Thus, the field line label we need for GS2 geometry quantities is

$$\alpha = \theta_v + \Lambda - \iota\zeta. \tag{33}$$

VMEC provides many quantities as functions of the coordinates (s, θ_v, ζ), where again $s = \psi/\psi_{LCFS}$. Specifically, it provides the Fourier amplitudes for expansions in θ_v and ζ, on grid points equally spaced in s. The quantities that are available include Λ, B, the cylindrical coordinates

(R, Z), the components

$$
\begin{aligned}
B^\theta &= \boldsymbol{B} \cdot \nabla \theta_v, \\
B^\zeta &= \boldsymbol{B} \cdot \nabla \zeta, \\
B_s &= \boldsymbol{B} \cdot \frac{\partial \boldsymbol{r}}{\partial s}, \\
B_\theta &= \boldsymbol{B} \cdot \frac{\partial \boldsymbol{r}}{\partial \theta_v}, \\
B_\zeta &= \boldsymbol{B} \cdot \frac{\partial \boldsymbol{r}}{\partial \zeta},
\end{aligned}
$$

and the Jacobian

$$
\sqrt{g} = \frac{\partial \boldsymbol{r}}{\partial s} \cdot \frac{\partial \boldsymbol{r}}{\partial \theta_v} \times \frac{\partial \boldsymbol{r}}{\partial \zeta} = \frac{1}{\nabla s \cdot \nabla \theta_v \times \nabla \zeta}. \tag{34}
$$

Here $\boldsymbol{r}(s, \theta_v, \zeta)$ is the position vector. Throughout this note, we will use $\sqrt{g}$ to denote the Jacobian of the non-straight-field-line VMEC coordinates, as in (34).

3 Computation of GS2 geometry quantities from VMEC data

Given the desired central flux surface ψ_0, and given a desired set of grid points in α and ζ, a 1D nonlinear root-finding algorithm is applied to solve (33) for the value of θ_v at each grid point. The `bmag` array is then obtained by evaluating B at the (θ_v, ζ) grid points, using VMEC's Fourier arrays `bmnc` and `bmns`.

For the full-flux-surface calculation, we will take the parallel coordinate z to be the toroidal angle ζ. Then to evaluate `gradpar`, we use

$$
\texttt{gradpar} = L_{ref} \frac{\boldsymbol{B} \cdot \nabla \zeta}{B} = L_{ref} \frac{B^\zeta}{B}, \tag{35}
$$

where B^ζ is available in the VMEC output through the variables `bsupvmnc` and `bsupvmns`.

To evaluate the quantities `gds*`, we must obtain the Cartesian components of $\nabla \psi$ and $\nabla \alpha$. To this end, we use the dual relations:

$$
\nabla s = \frac{1}{\sqrt{g}} \frac{\partial \boldsymbol{r}}{\partial \theta_v} \times \frac{\partial \boldsymbol{r}}{\partial \zeta}, \tag{36}
$$

$$
\nabla \theta_v = \frac{1}{\sqrt{g}} \frac{\partial \boldsymbol{r}}{\partial \zeta} \times \frac{\partial \boldsymbol{r}}{\partial s}. \tag{37}
$$

The right hand sides of these two expressions can be evaluated in terms of Cartesian components using the VMEC outputs `rmnc`, `rmns`, `zmnc`, and `zmns`, yielding Cartesian components for ∇s and $\nabla \theta_v$. Also the Cartesian components of $\nabla \zeta$ are known since ζ is the standard toroidal angle. We can then compute

$$
\nabla \psi = \frac{d\psi}{ds} \nabla s = \psi_{LCFS} \frac{1}{\sqrt{g}} \frac{\partial \boldsymbol{r}}{\partial \theta_v} \times \frac{\partial \boldsymbol{r}}{\partial \zeta} \tag{38}
$$

and

$$
\begin{aligned}
\nabla \alpha &= \nabla(\theta_v + \Lambda - \iota \zeta) \\
&= \left(\frac{\partial \Lambda}{\partial s} - \zeta \frac{d\iota}{ds} \right) \nabla s + \left(1 + \frac{\partial \Lambda}{\partial \theta_v} \right) \nabla \theta_v + \left(-\iota + \frac{\partial \Lambda}{\partial \zeta} \right) \nabla \zeta.
\end{aligned} \tag{39}
$$

Do we want to subtract `zeta_center` from ζ here so the secular ζ term in $\nabla\alpha$ vanishes at the center of the domain? Or might we want it to vanish somehwhere other than the center of the domain? Now that Cartesian components of $\nabla\psi$ and $\nabla\alpha$ are known, `gds2`, `gds21`, and `gds22` can be computed.

To evaluate `gbdrift0` = `cvdrift0`, we can use

$$\begin{aligned}
\boldsymbol{B}\times\nabla B\cdot\nabla\psi &= \boldsymbol{B}\times\nabla\zeta\cdot\nabla\psi\frac{\partial B}{\partial\zeta} + \boldsymbol{B}\times\nabla\theta_v\cdot\nabla\psi\frac{\partial B}{\partial\theta_v} \\
&= \left(B_\theta\nabla\theta_v\times\nabla\zeta\cdot\nabla s\frac{\partial B}{\partial\zeta} + B_\zeta\nabla\zeta\times\nabla\theta_v\cdot\nabla s\frac{\partial B}{\partial\theta_v}\right)\frac{d\psi}{ds} \\
&= \left(B_\theta\frac{\partial B}{\partial\zeta} - B_\zeta\frac{\partial B}{\partial\theta_v}\right)\frac{\psi_{LCFS}}{\sqrt{g}}. \qquad (40)
\end{aligned}$$

To obtain this result we have used

$$\nabla B = \frac{\partial B}{\partial s}\nabla s + \frac{\partial B}{\partial\theta_v}\nabla\theta_v + \frac{\partial B}{\partial\zeta}\nabla\zeta \qquad (41)$$

and

$$\boldsymbol{B} = B_s\nabla s + B_\theta\nabla\theta_v + B_\zeta\nabla\zeta. \qquad (42)$$

The quantity B_θ is available as the VMEC outputs `bsubumnc` and `bsubumns`, and the quantity B_ζ is available as the VMEC outputs `bsubvmnc` and `bsubvmns`.

A couple of options are possible for computing `gbdrift`. One method is to compute the Cartesian components of ∇B using (41) together with (36)-(37). Furthermore, the Cartesian components of $\boldsymbol{B}$ can be computed from

$$\begin{aligned}
\boldsymbol{B} &= \nabla\psi\times\nabla(\theta_v+\Lambda) + \iota\nabla\zeta\times\nabla\psi \\
&= \frac{d\psi}{ds}\left[\left(1+\frac{\partial\Lambda}{\partial\theta_v}\right)\nabla s\times\nabla\theta_v + \left(\iota-\frac{\partial\Lambda}{\partial\zeta}\right)\nabla\zeta\times\nabla s\right] \\
&= \frac{\psi_{LCFS}}{\sqrt{g}}\left[\left(1+\frac{\partial\Lambda}{\partial\theta_v}\right)\frac{\partial\boldsymbol{r}}{\partial\zeta} + \left(\iota-\frac{\partial\Lambda}{\partial\zeta}\right)\frac{\partial\boldsymbol{r}}{\partial\theta_v}\right]. \qquad (43)
\end{aligned}$$

Now that Cartesian components of $\boldsymbol{B}$, ∇B, and $\nabla\alpha$ are all known, their cross product needed for `gbdrift` is straightforward. Alternatively, `gbdrift` can be computed by substituting (41)-(42) and (39) into $\boldsymbol{B}\times\nabla B\cdot\nabla\alpha$, yielding

$$\begin{aligned}
\boldsymbol{B}\times\nabla B\cdot\nabla\alpha = \frac{1}{\sqrt{g}}\Bigg[&B_s\frac{\partial B}{\partial\theta_v}\left(\frac{\partial\Lambda}{\partial\zeta}-\iota\right) + B_\theta\frac{\partial B}{\partial\zeta}\left(\frac{\partial\Lambda}{\partial s}-\zeta\frac{d\iota}{ds}\right) + B_\zeta\frac{\partial B}{\partial s}\left(1+\frac{\partial\Lambda}{\partial\theta_v}\right) \\
&-B_\zeta\frac{\partial B}{\partial\theta_v}\left(\frac{\partial\Lambda}{\partial s}-\zeta\frac{d\iota}{ds}\right) - B_\theta\frac{\partial B}{\partial s}\left(\frac{\partial\Lambda}{\partial\zeta}-\iota\right) - B_s\frac{\partial B}{\partial\zeta}\left(1+\frac{\partial\Lambda}{\partial\theta_v}\right)\Bigg]. \qquad (44)
\end{aligned}$$

The last quantity we need to evaluate is `cvdrift`. Using

$$\begin{aligned}
\boldsymbol{B}\times\boldsymbol{\kappa} &= \boldsymbol{B}\times(\boldsymbol{b}\cdot\nabla\boldsymbol{b}) = \boldsymbol{B}\times[(\nabla\times\boldsymbol{b})\times\boldsymbol{b}] \\
&= \boldsymbol{B}\times\left[-\frac{1}{B^2}(\nabla B\times\boldsymbol{B})\times\boldsymbol{b} + \frac{\mu_0}{B^2}\boldsymbol{j}\times\boldsymbol{B}\right] \\
&= \frac{1}{B}\boldsymbol{B}\times\nabla B + \frac{\mu_0}{B^2}\frac{dp}{ds}\boldsymbol{B}\times\nabla s, \qquad (45)
\end{aligned}$$

(where we have used the MHD equilibrium equation $\boldsymbol{j} \times \boldsymbol{B} = \nabla p$), we find

$$\texttt{cvdrift} = \texttt{gbdrift} + \frac{2B_{ref}L_{ref}^2}{B^2}\sqrt{\frac{\psi}{\psi_{LCFS}}}\frac{\mu_0}{B^2}\frac{dp}{ds}\boldsymbol{B} \times \nabla s \cdot \nabla \alpha. \tag{46}$$

In the last term, $\boldsymbol{B} \times \nabla s \cdot \nabla \alpha$ can either be evaluated using the Cartesian components of $\boldsymbol{B}$, ∇s, and $\nabla \alpha$, the calculation of which has already been described, or by combining (39) and (42) to obtain

$$\boldsymbol{B} \times \nabla s \cdot \nabla \alpha = \frac{1}{\sqrt{g}}\left[B_\zeta\left(1 + \frac{\partial \Lambda}{\partial \theta_v}\right) - B_\theta\left(\frac{\partial \Lambda}{\partial \zeta} - \iota\right)\right]. \tag{47}$$

4 Parallel boundary condition and wavenumber quantization for a full surface calculation

Let us now consider a full-flux-surface calculations, using field-aligned coordinates. We continue to use ψ and α as perpendicular coordinates, and ζ as the third (parallel) coordinate. In a full-flux-surface calculation, the range of α is $[0,\ 2\pi)$, which can be seen from the fact at fixed ψ and ζ, the 2π-periodicity of quantities in θ_p implies 2π-periodicity in α.

Just as in a flux tube code, fluctuating quantities such as the electrostatic potential ϕ are represented as

$$\phi(\psi, \alpha, \zeta) = \sum_{k_\psi, k_\alpha} \bar{\phi}_{k_\psi, k_\alpha}(\zeta) \exp\left(ik_\alpha \alpha + ik_\psi \left[\psi - \psi_0\right]\right). \tag{48}$$

Again, ψ_0 indicates the flux surface about which the numerical domain is centered. The wavenumbers with respect to (ψ, α) are related to wavenumbers with respect to (x, y) through

$$\begin{aligned} k_x &= k_\psi \frac{d\psi}{dx}, \\ k_y &= k_\alpha \frac{d\alpha}{dy}. \end{aligned} \tag{49}$$

Note that k_α ranges over the integers, due to the 2π-periodicity in α discussed above. The choice of y (19) then implies the wavenumber grid in y must be

$$k_y \rho_{ref} = \frac{\rho_{ref}}{L_{ref}\sqrt{s(\psi_0)}} \times (\text{integers}). \tag{50}$$

We take fluctuating quantities to be periodic in ψ, just as in a flux tube code. The allowed values of k_ψ and associated 'box size' in ψ will be derived below.

We take fluctuating quantities to be periodic in ζ with period $2\pi P$ at fixed ψ and θ_p. Here, P is a rational number, typically the inverse of the number of field periods (e.g. 5 for W7-X). One could also choose $P = 1$ to simulate the entire toroidal domain, or choose $P =$ integer / (number of field periods) for an intermediate domain size. When $P = 1$, this periodicity condition is the true periodicity of the torus. When $P =$ integer / (number of field periods), the periodicity imposed in the code is effectively a statement of statistical periodicity of the turbulence at geometrically equivalent points in the domain. To see the implications of imposing periodicity in ζ at fixed θ_p, we substitute $\alpha = \theta_p - \iota\zeta$ and the Taylor expansion

$$\iota \approx \iota(\psi_0) + \frac{d\iota}{d\psi}\left[\psi - \psi_0\right] \tag{51}$$

into (48). (We take $d\iota/d\psi$ to be evaluated at ψ_0, and hence constant over the domain.) The result is

$$\phi = \sum_{k_\psi,k_\alpha} \bar{\phi}_{k_\psi,k_\alpha}(\zeta) \exp\left(ik_\alpha\theta_p - ik_\alpha\iota(\psi_0)\zeta + i\left[-k_\alpha \frac{d\iota}{d\psi}\zeta + k_\psi \right] [\psi - \psi_0] \right). \tag{52}$$

When a particular (k_ψ, k_α) Fourier mode gets to the end of the ζ domain ($\zeta = 2\pi P$), we want the mode to connect exactly to another Fourier mode in the simulation (k'_ψ, k'_α), with the latter evaluated at $\zeta = 0$. Mathematically, this condition is

$$\begin{aligned} &\bar{\phi}_{k_\psi,k_\alpha}(2\pi P) \exp\left(ik_\alpha\theta_p - ik_\alpha\iota(\psi_0)2\pi P + i\left[-k_\alpha \frac{d\iota}{d\psi}2\pi P + k_\psi \right] [\psi - \psi_0] \right) \\ &= \bar{\phi}_{k'_\psi,k'_\alpha}(0) \exp\left(ik'_\alpha\theta_p + ik'_\psi [\psi - \psi_0] \right). \end{aligned} \tag{53}$$

For this equation to hold for all θ_p at fixed ψ, we must have $k'_\alpha = k_\alpha$. For equality to hold for all ψ at fixed θ_p, we must have

$$k'_\psi = k_\psi - k_\alpha \frac{d\iota}{d\psi} 2\pi P. \tag{54}$$

This last result is analogous to the twist-and-shift condition used in flux-tube GS2. If k'_ψ is to be included in the wavenumber grid, and assuming the k_ψ grid consists of integer multiples of some $k_{\psi,min}$, then the difference $k'_\psi - k_\psi$ should be an integer multiple of $k_{\psi,min}$. In particular this must be true for the smallest nonzero k_α, which is 1. Thus, we conclude

$$\frac{d\iota}{d\psi} 2\pi P = (\texttt{jtwist}) k_{\psi,min} \tag{55}$$

where `jtwist` is an integer. It follows that the 'box size' in ψ, denoted L_ψ, is

$$L_\psi = \frac{2\pi}{k_{\psi,min}} = \frac{(\texttt{jtwist})}{P} \left(\frac{d\iota}{d\psi} \right)^{-1}. \tag{56}$$

Using (49) and (18), the equivalent box size in x is

$$L_x = \frac{dx}{d\psi} L_\psi = \frac{2\pi}{k_{x,min}} = \frac{(\texttt{jtwist})}{P L_{ref} B_{ref} \sqrt{s}} \left(\frac{d\iota}{d\psi} \right)^{-1}. \tag{57}$$

Unfortunately, in low-shear stellarators like W7-X and HSX, $d\iota/d\psi$ in (57) can be quite small, meaning L_x must be quite large.

Equation (53) also indicates there should be a phase shift when two Fourier modes are connected:

$$\bar{\phi}_{k_\psi,k_\alpha}(2\pi P) \exp\left(-ik_\alpha\iota(\psi_0)2\pi P \right) = \bar{\phi}_{k'_\psi,k_\alpha}(0). \tag{58}$$

4.1 Continuity of geometric quantities

We can verify that various terms in the gyrokinetic equation are continuous across the parallel boundary condition. First, let us consider the magnetic drift term:

$$\begin{aligned}\boldsymbol{v}_m \cdot \nabla h &= \boldsymbol{v}_m \cdot \nabla \left[\sum_{k_\psi,k_\alpha} \bar{h}_{k_\psi,k_\alpha}(\zeta) \exp\left(ik_\alpha \alpha + ik_\psi[\psi-\psi_0]\right)\right] \\ &\approx \sum_{k_\psi,k_\alpha} \bar{h}_{k_\psi,k_\alpha}(\zeta) \exp\left(ik_\alpha \alpha + ik_\psi[\psi-\psi_0]\right) \left[ik_\alpha \boldsymbol{v}_m \cdot \nabla\alpha + ik_\psi \boldsymbol{v}_m \cdot \nabla\psi\right] \\ &= \sum_{k_\psi,k_\alpha} \bar{h}_{k_\psi,k_\alpha}(\zeta) \exp\left(ik_\alpha [\theta_p - \iota\zeta] + ik_\psi[\psi-\psi_0]\right) \\ &\qquad \times \left[ik_\alpha \boldsymbol{v}_m \cdot \left(\nabla\theta_p - \iota\nabla\zeta - \zeta\frac{d\iota}{d\psi}\nabla\psi\right) + ik_\psi \boldsymbol{v}_m \cdot \nabla\psi\right], \end{aligned} \tag{59}$$

where h is the nonadiabatic distribution function. (The $\approx$ above comes from dropping the slow ζ dependence of $\bar{h}_{k_\psi,\zeta}$ in the gradient.) As ζ is increased, just before the boundary $\zeta = 2\pi P$ we have

$$\begin{aligned}(\boldsymbol{v}_m \cdot \nabla h)_- = &\sum_{k_\psi,k_\alpha} \bar{h}_{k_\psi,k_\alpha}(2\pi P) \exp\left(ik_\alpha [\theta_p - \iota 2\pi P] + ik_\psi[\psi-\psi_0]\right) \\ &\times \left[ik_\alpha \boldsymbol{v}_m \cdot \left(\nabla\theta_p - \iota\nabla\zeta - 2\pi P\frac{d\iota}{d\psi}\nabla\psi\right) + ik_\psi \boldsymbol{v}_m \cdot \nabla\psi\right]. \end{aligned} \tag{60}$$

The subscript on the left hand side indicates that we have evaluated the result just to the left of the boundary. On the other side of the boundary ($\zeta = 0$), (59) evaluates to

$$(\boldsymbol{v}_m \cdot \nabla h)_+ = \sum_{k_\psi,k_\alpha} \bar{h}_{k'_\psi,k_\alpha}(0) \exp\left(ik_\alpha \theta_p + ik'_\psi[\psi-\psi_0]\right) \left[ik_\alpha \boldsymbol{v}_m \cdot (\nabla\theta_p - \iota\nabla\zeta) + ik'_\psi \boldsymbol{v}_m \cdot \nabla\psi\right]. \tag{61}$$

In this last equation, we were free to put primes on k_ψ because it is summed over. Applying (54) and (58),

$$\begin{aligned}(\boldsymbol{v}_m \cdot \nabla h)_+ = &\sum_{k_\psi,k_\alpha} \bar{h}_{k_\psi,k_\alpha}(2\pi P) \exp\left(ik_\alpha\theta_p - ik_\alpha\iota(\psi_0)2\pi P + i\left[k_\psi - k_\alpha\frac{d\iota}{d\psi}2\pi P\right][\psi-\psi_0]\right) \\ &\times \left[ik_\alpha \boldsymbol{v}_m \cdot (\nabla\theta_p - \iota\nabla\zeta) + i\left[k_\psi - k_\alpha\frac{d\iota}{d\psi}2\pi P\right] \boldsymbol{v}_m \cdot \nabla\psi\right]. \end{aligned} \tag{62}$$

Using (51), it can be seen that (60) is identical to (62), so the magnetic drift term is indeed continuous across the boundary.

Also show continuity for $\langle\phi\rangle_R$...