Existence and calculation of sharp boundary magnetohydrodynamic equilibrium in three-dimensional toroidal geometry

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The problem of sharp boundary, ideal magnetohydrodynamic equilibria in three-dimensional toroidal geometry is addressed. The sharp boundary, which separates a uniform pressure, current-free plasma from a vacuum, is determined by a magnetic surface of a given vacuum magnetic field. The pressure balance equation has the form of a Hamilton–Jacobi equation with a Hamiltonian that is quadratic in the momentum variables, which are the two covariant components of the magnetic field on the outer surface of the plasma. The condition of finding a unique solution on the outer surface is identical with finding phase-space tori in nonlinear dynamics problems, and the Kolmogorov–Arnold–Moser (KAM) theorem guarantees that such solutions exist for a wide band of parameters. Perturbation theory is used to calculate the properties of the magnetic field just outside the plasma. Special perturbation theory is needed to treat resonances and it is explicitly shown that there are bands of pressure where there are no solutions.

I. INTRODUCTION

The purpose of this work is to establish a method for solving the fully three-dimensional sharp boundary, ideal magnetohydrodynamic (MHD) equilibrium equations in toroidal geometry. The sharp boundary model has frequently been used to obtain the gross equilibrium[1,2] and stability[1,3,4] structure of toroidal configurations. To our knowledge, the existence of such an equilibrium in fully three-dimensional geometry[5] has not been demonstrated previously. Here we develop a method that poses and solves the sharp boundary equilibria model. We are able to show that sharp boundary equilibria exist in a fully three-dimensional vacuum configuration if an appropriate "time-separated" two-dimensional Hamilton–Jacobi equation for the action function has single-valued solutions for the space derivatives of the action. This type of condition has also been specified by Grad[6] and independently by Wobig[7] for equilibria where the entire magnetic field is excluded (beta equals 1) in the finite pressure region. Numerical calculations for fully three-dimensional sharp boundary equilibria have been attempted by Meyer and Schmitt[8] for beta equals 1 plasmas and by Betancourt and Garabedian[2] for beta less than 1 plasmas. In this paper we show that the Hamilton–Jacobi equation has single-valued solutions for fully three-dimensional configurations if beta is sufficiently small.

II. SHARP BOUNDARY MODEL

We develop sharp boundary equilibria in terms of a vacuum magnetic field $\mathbf{B}_v$, which is generated by a suitable distribution of external currents. The field $\mathbf{B}_v$ is assumed to have a toroidal magnetic surface S, that is, a surface to which the field lines are everywhere tangential, that the field lines on this surface have an irrational rotational transform, and that there are no vacuum currents inside. A somewhat more general definition for a vacuum surface can be formulated for field lines that close on themselves, but our definition suffices for the purpose of this paper. Having such a surface means that the surface S can be generated from a point $\mathbf{r} = \mathbf{r}_0$ on S by obtaining the solution of the equation

$$\frac{d\mathbf{r}}{ds} = \frac{\mathbf{B}_v}{|\mathbf{B}_v|},$$

where s is the distance along a field line. The existence of such a vacuum flux surface has been proved rigorously for configurations that can be treated as perturbations from helical symmetry.[9,10] Vacuum magnetic flux surfaces are believed to exist when perturbations from symmetry are finite. This existence question is discussed further in the Appendix.

Now we consider a sharp boundary equilibrium that consists of a constant plasma pressure profile with zero current inside the surface S and zero pressure outside the surface. The magnetic field $\mathbf{B}_p$ inside the surface S must then be given by

$$\mathbf{B}_p = \lambda\, \mathbf{B}_v ,$$

where λ is a constant, as then

$$\nabla \times \mathbf{B}_p = 0$$

and

$$\mathbf{B}_p \cdot \hat{\mathbf{n}} = 0 ,$$

where $\hat{\mathbf{n}}$ is a unit vector normal to the surface. The value of the proportionality constant λ is related to the total external poloidal current linking the surface S (the poloidal currents are carried by vacuum coils outside S, as well as plasma surface current on S, and for definiteness the total vacuum poloidal current is taken to be $2\pi g$). Outside S one has to find the magnetic field $\mathbf{B}_e$ ($\mathbf{B}_e \neq \mathbf{B}_v$ except for the degenerate case of zero pressure and zero surface current on S).

The existence of finite pressure equilibria in this state requires that two conditions be satisfied: (i) that the plasma–vacuum interface S be a magnetic surface for not only the internal plasma magnetic field $\mathbf{B}_p$ but also for the external vacuum magnetic field $\mathbf{B}_e$; (ii) that pressure balance be

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maintained across S, i.e., $2p_0 = B_e^2 - B_p^2$, where p_0 is the plasma pressure. Given p_0 and $\mathbf{B}_p$, the essential problem is to show that the solutions for $\mathbf{B}_e$ are single valued at every point on the surface S.

The magnetic field $\mathbf{B}_v$, in the enclosed vacuum region bounded by S, is derivable from a scalar potential Φ_v that satisfies Laplace's equation. This potential is subject to the conditions that the normal component of $\mathbf{B}_v$ vanishes on S and that Φ_v changes by a fixed value in one toroidal circuit. These conditions define a well-posed Neumann problem for Φ_v:

$$\nabla^2\Phi_v = 0 \text{ inside } S, \quad \hat{\mathbf{n}}\cdot\nabla\Phi_v = 0 \text{ on } S,$$
$$\Phi_v(\varphi = 2\pi) - \Phi_v(\varphi = 0) = C, \tag{1}$$

where $\hat{\mathbf{n}}$ is a normal vector on S, φ is a toroidal-like angle, and C is a specified constant, which physically is the linked poloidal current. By assumption, $\Phi_v(\mathbf{r})$ defines a magnetic field on S that has an irrational rotational transform.

To represent the field $\mathbf{B}_v$, it is convenient to adopt the covariant and contravariant notation that has been emphasized by Boozer[11] (although the Hamiltonian structure to be described is independent of the coordinates chosen):

$$\mathbf{B}_v = \nabla\Phi_v = \nabla\alpha_v \times \nabla\beta_v \,. \tag{2}$$

We note that even if only one magnetic surface exists, $\nabla\alpha_v$ and $\nabla\beta_v$ can be constructed on that surface as discussed in Ref. 12. The surface is denoted by $\alpha_v = \text{const}$, where α_v is the enclosed toroidal flux divided by 2π, and β_v then varies from zero to 2π in a poloidal transit at constant Φ_v.[11] If one introduces poloidal and toroidal angular coordinates, θ and ϕ, respectively, one has the expressions

$$\beta_v = \theta - x(\alpha_v)\phi, \quad \Phi_v = g\phi\,, \tag{3}$$

where $x(\alpha_v)$ is the rotational transform of $\mathbf{B}_v$ on the flux surface labeled by α_v, and $2\pi g$ is the total enclosed poloidal current.[11] The triad $(\Phi_v, \alpha_v, \beta_v)$ provides a label of all spatial points on a given flux surface. All functions can be expressed in terms of these three variables. Since the vacuum magnetic fields generate an exact surface S, we can use convergent Fourier series expressions in the coordinates β_v and Φ_v. In particular, below we will use the following:

$$\frac{1}{B_v^2} = \frac{1}{B_0^2} + \sum_{m,n=-\infty}^{\infty} \frac{\delta_{m,n}}{B_0^2} \exp\left(\frac{i(n - mx)}{g}\Phi_v - im\beta_v\right)$$
$$\equiv \frac{1}{B_0^2}[1 + \delta(\Phi_v,\beta_v)]\,, \tag{4}$$

$$\frac{1}{|\nabla\alpha_v|^2} = \frac{1}{|\nabla\alpha_v|_0^2} + \sum_{m,n=-\infty}^{\infty} \frac{\alpha_{m,n}}{|\nabla\alpha_v|_0^2}$$
$$\times\exp\left(\frac{i(n-mx)}{g}\Phi_v - im\beta_v\right) \equiv \frac{1 + \alpha(\Phi_v,\beta_v)}{|\nabla\alpha_v|_0^2}, \tag{5}$$

where B_0^2, $\delta_{m,n}$, $\alpha_{m,n}$, x, $|\nabla\alpha_v|_0^2$ are functions only of α_v, $\delta_{-m,-n} = \delta^*_{m,n}$, $\alpha_{-m,-n} = \alpha^*_{m,n}$, and $\delta_{0,0} = \alpha_{0,0} = 0$. Frequently, the symmetry of the problem is such that a phase can be chosen so that $\delta_{m,n}$ and $\alpha_{m,n}$ are real. We shall assume $1/B_v^2$ and $1/|\nabla\alpha_v|^2$ are analytic functions of the surface variables. In order for these functions to have surface derivatives of arbitrary order, $\alpha_{m,n}$ and $\delta_{m,n}$ must converge exponentially for large m and n. We note that even if we consider a system where the vacuum surface S is close to being destroyed (e.g., when S is in the neighborhood of spatial regions where the vacuum magnetic field is ergodic) the $\alpha_{m,n}$ sequence should still vanish exponentially as is indicated in analyticity studies of somewhat similar nonlinear Hamiltonian map problems.[13]

We now attempt to find a sharp boundary equilibrium on the surface S, which is defined by $\alpha_v = \text{const}$. In the volume A enclosed by S, there is pressure p_0, while the total external poloidal current just outside S is $2\pi g$. As noted earlier, the magnetic field in A is taken as

$$\mathbf{B}_p = \lambda\,\mathbf{B}_v\,, \tag{6}$$

where λ is a constant that depends parametrically on p_0. Hence $\nabla\times\mathbf{B}_p = 0$ in region A. Across S there is a pressure jump that is governed by the relationship

$$B_e^2 = \lambda^2 B_v^2 + 2p_0\,, \tag{7}$$

where $\mathbf{B}_e$ is the magnetic field just outside S. We can represent $\mathbf{B}_e$ in terms of a scalar $\Phi'(\Phi_v,\alpha_v,\beta_v)$ as

$$\mathbf{B}_e = \nabla\Phi' = \frac{\partial\Phi'}{\partial\Phi_v}\nabla\Phi_v + \frac{\partial\Phi'}{\partial\alpha_v}\nabla\alpha_v + \frac{\partial\Phi'}{\partial\beta_v}\nabla\beta_v\,. \tag{8}$$

Since the normal component of the magnetic field is zero on either side of S, we impose the condition $\mathbf{B}_e\cdot\nabla\alpha_v = 0$, which in turn implies the relationship

$$\frac{\partial\Phi'}{\partial\alpha_v} = -\frac{\partial\Phi'}{\partial\beta_v}\frac{\nabla\alpha_v\cdot\nabla\beta_v}{|\nabla\alpha_v|^2} \tag{9a}$$

and

$$\mathbf{B}_e = \frac{\partial\Phi'}{\partial\Phi_v}\mathbf{B}_v + \frac{\partial\Phi'}{\partial\beta_v}\frac{\mathbf{B}_v\times\nabla\alpha_v}{|\nabla\alpha_v|^2}\,. \tag{9b}$$

Now, combining Eqs. (7), (8), and (9) yields the following expression for pressure balance across S:

$$1 + 2p/B_0^2 = 2H(\Phi_v,\beta_v) \tag{10}$$

with

$$H = \frac{1}{2}\left(\frac{\partial\Phi(\Phi_v,\beta_v)}{\partial\Phi_v}\right)^2 + \frac{1}{2}\left(\frac{\partial\Phi(\Phi_v,\beta_v)}{\partial\beta_v}\right)^2\frac{1}{|\nabla\alpha_v|_0^2}$$
$$\times[1 + \alpha(\Phi_v,\beta_v)] - (p/B_0^2)\delta(\Phi_v,\beta_v)\,, \tag{11}$$

where we have rescaled Φ' and p_0 so that $\Phi(\Phi_v,\beta_v) = \Phi'/\lambda$, $p = p_0/\lambda^2$. Equation (10) is in the form of a first-order nonlinear partial differential equation for the potential $\Phi(\Phi_v,\beta_v)$, which can be solved by the method of characteristics. This equation also has the form of a time-separated Hamilton–Jacobi equation where Φ is Hamilton's characteristic function. By introducing the notation $P_\phi = \partial\Phi/\partial\Phi_v$ and $P_\beta = \partial\Phi/\partial\beta_v$, H in Eq. (10) is seen to be the Hamiltonian of a two degree of freedom autonomous system where the system's "energy" is $\frac{1}{2} + p/B_0^2$. The Hamiltonian system given by Eq. (11) resembles a conventional dynamics problem of a particle in a potential when non-Euclidean coordinates are used.

The equations determining the characteristics are now of the form of Hamilton's equations

$$\frac{dP_\phi}{dt} = -\frac{\partial H}{\partial \Phi_v}, \quad \frac{dP_\beta}{dt} = -\frac{\partial H}{\partial \beta_v},$$
$$\frac{d\Phi_v}{dt} = \frac{\partial H}{\partial P_\phi}, \quad \frac{d\beta_v}{dt} = \frac{\partial H}{\partial P_\beta}, \tag{12}$$

where the Hamiltonian H is given by Eq. (10) and is now considered to be a function of β_v, Φ_v, P_β, and P_ϕ. Along the characteristics $\Phi_v = \Phi_v(t)$ and $\beta_v = \beta_v(t)$, the potential $\Phi(t)$ is governed by the expression

$$\frac{d\Phi}{dt} = P_\phi \frac{d\Phi_v}{dt} + P_\beta \frac{d\beta_v}{dt}. \tag{13}$$

In the canonical system of Eqs. (12), the effective time parameter has no particular physical meaning. However, the characteristic function Φ has a very important physical meaning in that it determines λ via the expression

$$\lambda = 2\pi g/\Delta\Phi_{\rm tor}, \tag{14}$$

where $\Delta\Phi_{\rm tor}$ is the jump in Φ upon returning to the same spatial point on S after one toroidal transit and no poloidal transits. From the jump in Φ in one poloidal transit and no toroidal transits, denoted by $\Delta\Phi_{\rm pol}$, one finds that the toroidal current $I_{\rm tor}$ on the surface S is

$$I_{\rm tor} = 2\pi g(\Delta\Phi_{\rm pol}/\Delta\Phi_{\rm tor}). \tag{15}$$

It is well known that a complete solution of the two-dimensional Hamilton–Jacobi equation [Eqs. (10)] involves two constants, which are conveniently expressed in terms of the "actions" $\Delta\Phi_{\rm pol}$ and $\Delta\Phi_{\rm tor}$.

We note that the lines of force of $\mathbf{B}_e$ on S can be identified with the trajectories determined from Eqs. (12). This follows from Eq. (7), which can be written in the form $\mathbf{B}_e \cdot \nabla\Phi' = \lambda^2 B_v^2 + 2p_0$. The characteristics of this partial differential equation are given by $\mathbf{r} = \mathbf{r}(t')$, where $\mathbf{r}(t')$ satisfies a nonlinear ordinary differential equation, $(d\mathbf{r}/dt') = \mathbf{B}_e$. Consequently, the position vector $\mathbf{r} = \mathbf{r}(t')$ traces out the lines of force of $\mathbf{B}_e$.

In order to generate an equilibrium, the solution to Eq. (12) must have the periodicity property that for some initial values, $P_{\phi 0}$ and $P_{\beta 0}$, at a point on S with coordinates Φ_{v0} and β_{v0}, a *single-valued* solution for P_ϕ and P_β is generated at every point on S, i.e., $P_\phi(\Phi_v + 2\pi g, \beta_v - 2\pi x) = P_\phi(\Phi_v, \beta_v)$. We note that upon specification of P_ϕ, Φ_v, and β_v, P_β^2 is determined by Eq. (10) as H is conserved. However, in general, the solution for P_ϕ is a multi-valued function of Φ_v and β_v, which can exhibit phase-space islands or an ergodic character as has been demonstrated in many examples of Hamiltonian nonlinear dynamics (e.g., see Refs. 14 and 15). Nevertheless, under certain conditions a large class of single-valued solutions for P_ϕ and P_β exist; this can be demonstrated by invoking the KAM theorem.[15] (We emphasize that here we apply the KAM theorem in a new context, viz., that of finding single-valued solutions for the momenta P_ϕ and P_β, in contrast to the use of the KAM theorem in Refs. 9 and 10 to assure the existence of vacuum magnetic flux surfaces when symmetry is broken.) To apply the theorem we shall transform the Hamiltonian given in Eq. (10) to one that is quadratic in momentum variables correct to $O(\epsilon^2)$, where

$$\epsilon \approx \frac{\alpha_{\max}^{1/2} P_\beta}{|\nabla\alpha_v|_0} \approx \left(p\,\frac{\delta_{\max}}{B_0^2}\right)^{1/2}.$$

Here $\alpha_{\max}$ is the upper bound of $|\alpha(\Phi_v, \beta_v)|$. To find the transformation we note that the time-separated Hamilton–Jacobi equation is

$$H = \frac{1}{2}\left(\frac{\partial\Phi}{\partial\Phi_v}(\Phi_v,\beta_v)\right)^2 + \frac{1}{2|\nabla\alpha_v|_0^2}\left(\frac{\partial\Phi}{\partial\beta_v}(\Phi_v,\beta_v)\right)^2 \times\left(1 + \sum_{m,n}\alpha_{m,n}\exp(i\psi_{m,n})\right) - \frac{p}{B_0^2}\sum_{m,n}\delta_{m,n}\exp(i\psi_{m,n}), \tag{16}$$

where $\psi_{m,n} = (n - mx)\Phi_v/g - m\beta_v$. This equation could also be written in terms of the toroidal and poloidal coordinates Φ_v and θ defined by Eq. (3). See the Appendix.

Now consider the canonical transformation

$$\tilde\Phi_v = \Phi_v + \sum_{m,n}\frac{\partial\gamma_{m,n}}{\partial\tilde P_\phi}e^{i\psi_{m,n}}, \tag{17a}$$

$$\tilde\beta_v = \beta_v + \sum_{m,n}\frac{\partial\gamma_{m,n}}{\partial\tilde P_\beta}e^{i\psi_{m,n}}, \tag{17b}$$

$$P_\phi = \tilde P_\phi + \sum_{m,n} i\left(\frac{n-mx}{g}\right)\gamma_{m,n}e^{i\psi_{m,n}}, \tag{17c}$$

$$P_\beta = \tilde P_\beta - \sum_{m,n} im\gamma_{m,n}e^{i\psi_{m,n}}, \tag{17d}$$

where we assume $\gamma_{m,n}$ is a function of $\tilde P_\phi$ and $\tilde P_\beta$ and independent of the coordinates. [The transformation in Eqs. (17) is derivable from a mixed variable generating function.] Substituting Eqs. (17) into Eq. (16) yields

$$H = \frac{1}{2}\tilde P_\phi^2 + \frac{\tilde P_\beta^2}{2|\nabla\alpha_v|_0^2} + \sum_{m,n}\left[i\tilde P_\phi\left(\frac{n-mx}{g}\right)\gamma_{m,n} + \frac{\alpha_{m,n}}{2|\nabla\alpha_v|_0^2}\tilde P_\beta^2 - \frac{p}{B_0^2}\delta_{m,n}\right]e^{i\psi_{m,n}} + \cdots. \tag{18}$$

If we choose,

$$\gamma_{m,n} = i\left(\frac{\tilde P_\beta^2 g\alpha_{m,n}}{2\tilde P_\phi(n-mx)|\nabla\alpha_v|_0^2} - \frac{p\delta_{m,n}g}{B_0^2(n-mx)\tilde P_\phi}\right), \tag{19}$$

then using $\tilde P_\phi \approx 1$ we see that the $\gamma_{m,n} = O(\epsilon^2)$ and the lowest-order Hamiltonian is

$$H = \tilde P_\phi^2/2 + \tilde P_\beta^2/2|\nabla\alpha_v|_0^2 + \cdots. \tag{20}$$

The Hamiltonian possesses four additional terms beside the kinetic energy terms of Eq. (20). These are $O[\gamma_{m,n}^2(n-mx)^2/g^2]$, $O(m^2\gamma_{m,n}^2/2|\nabla\alpha_v|_0^2)$, $O(\tilde P_\beta m\gamma_{m,n}\alpha_{m,n}/|\nabla\alpha_v|_0^2)$, and $O(m^2\gamma_{m,n}^2\alpha_{m,n}/2|\nabla\alpha_v|_0^2)$. We require each of these to be small compared to $\tilde P_\beta^2/2|\nabla\alpha_v|_0^2$. This yields a set of inequalities, the most stringent of which comes from the term $O(m^2\gamma_{m,n}^2/2|\nabla\alpha_v|_0^2)$. Equation (20) is in error by terms of $O(\epsilon^3)$ and thus to leading order $\tilde P_\phi$ and $\tilde P_\beta$ are constants, provided

$$\left|\frac{2|\nabla\alpha_v|_0^2(n-mx)}{gm\alpha_{m,n}}\right| > |\tilde{P}_\beta| > \left|\frac{mpg\delta_{m,n}}{B_0^2(n-mx)}\right| . \tag{21a}$$

It can be shown that the failure of the left-hand inequality in Eq. (21a) is associated with islands induced by a modification of the vacuum equilibrium caused by toroidal current on the flux surfaces, while the failure of the right-hand inequality is associated with islands induced by adding pressure inside the surface S. The interval for $\tilde{P}_\beta$ required by Eq. (21a) can always be found, provided

$$\frac{p|\delta_{m,n}\alpha_{m,n}|g^2m^2}{2B_0^2(n-mx)^2|\nabla\alpha_v|_0^2} \ll 1 . \tag{21b}$$

When this condition is satisfied, the island chains associated with toroidal current and pressure can simultaneously be treated perturbatively. It is clear that if $\delta_{m,n}$ approaches zero sufficiently rapidly as m and n approach ∞, and x is irrational (e.g., see Refs. 5, 14, and 15), this condition will be satisfied for the expansion parameter $p\delta_{\max}/B_0^2$ sufficiently small. Then, the external magnetic field of the form

$$\mathbf{B}_e = \frac{2\pi g}{\Delta\Phi_{\text{tor}}}\left(P_\phi \mathbf{B}_v + \frac{\mathbf{B}_v \times \nabla\alpha_v}{|\nabla\alpha_v|^2} P_\beta\right)$$

is determined just outside S.

Once the magnetic field is known on the outer plasma interface, one can calculate the required vacuum currents in a volume V outside S, which, together with the plasma surface current, generates the magnetic field $\mathbf{B}_e$ on S. Although the currents in V are not unique, the magnetic fields that they generate in the vicinity of S are unique. A set of currents can be calculated to arbitrary accuracy using the theory explained in Ref. 16.

Thus we have shown that the existence of an equilibrium to the sharp boundary stellarator model is tantamount to demonstrating that Eqs. (12) possess unique solutions for P_ϕ and P_β on the surface S. Since the Hamiltonian has a lowest-order form independent of coordinates, which is given by Eq. (20), it follows from the KAM theorem that for sufficiently small $p\delta_{\max}/B_0^2$ that there is a band of initial conditions, around small P_β, leading to single-valued solutions of Eqs. (12) with a measure approaching unity.

For a given spectrum of $\delta_{m,n}$ and $\alpha_{m,n}$, one can attempt to find a periodic solution of Eq. (12) numerically. If one starts with initial values for the variables P_ϕ, P_β, Φ_v, and β_v [the pressure p is determined from Eq. (10)], one can ascertain with surface of section plots, of say P_β vs β_v at $\Phi_v = 2\pi gr$ with r an integer, whether single-valued solutions are attained. If this happens, the $\lambda \equiv 2\pi g/\Delta\Phi_{\text{tor}}$, and the enclosed toroidal current is

$$I_{\text{tor}} = 2\pi g(\Delta\Phi_{\text{pol}}/\Delta\Phi_{\text{tor}}) .$$

When I_{tor} and p are given, one can attempt to satisfy this equation by iteration of initial values.

III. ANALYTIC CALCULATIONS

Let us now assume that $p\delta_{\max}/B_0^2 \approx \epsilon \ll 1$ and demonstrate how analytic solutions can be obtained (we will use this altered definition of ϵ in the remainder of the paper). For definiteness we shall search for solutions where the total enclosed toroidal current is small. We assume the following form for the solution of Eq. (10):

$$\Phi = a\Phi_v + ax_c|\nabla\alpha_v|_0^2\beta_v/g + \Phi_1(\Phi_v,\beta_v) ,$$

where a and x_c are constants and $a\,\partial\Phi_1/\partial\Phi_v \approx x_c/a = O(\epsilon)$. We also note from Eq. (14) that

$$1/a = (1 - xx_c|\nabla\alpha_v|_0^2/g^2)\lambda_0(p) \equiv \mu\lambda_0(p) , \tag{22}$$

where λ_0 is the value of λ with resonances neglected. As p increases, the rotational transform of the external field $\mathbf{B}_e$ will change. At some value of pressure, we isolate the resonant term with (N/M) closest to the rotational transform $x(p)$ of $\mathbf{B}_e$. The sums in Eqs. (4) and (5) can be divided into a sum of nonresonant terms plus one resonant term. For example, Eq. (4) can be rewritten

$$\frac{p}{B_v^2} = \frac{p}{B_0^2} + \sum_{m,n}{}' \frac{p\delta_{m,n}}{B_0^2}\exp\left(\frac{i(n-mx)}{g}\Phi_v - im\beta_v\right) + \frac{p}{B_0^2}\sum_r \delta_{rM,rN}\exp(-irM\psi')$$

$$\equiv (p/B_0^2)[1 + \delta_N(\Phi_v,\beta_v) + \delta_R(M\psi')] , \tag{23}$$

where $\psi' = \beta_v - (N/M - x)\Phi_v/g$, and the primed sum excludes the resonance terms $(m,n) = (rM,rN)$ with r an integer.

We define $x_0(p)$ as the rotational transform in the absence of the resonant term $\delta_{rM,rN}$. We then renormalize the β_v coordinate by seeking a transformation,

$$\beta_v = \beta_0 + \beta_1(\Phi_v,\beta_v;p) = \beta_0 + \delta\beta_1(\Phi_v,\beta_v;p) + [x_0(p) - x]\Phi_v/g , \tag{24}$$

for which $(d\beta_0/dt) = 0$ in the absence of the resonant contributions $\delta_{rM,rN}$, $\alpha_{rM,rN}$ and other higher-order resonant mode coupling terms in the Hamiltonian given by Eq. (10) (we will not calculate to a high enough order to treat the higher-order resonant terms). Also, in Eq. (24) $\delta\beta_1$ is nonsecular. The transformation can be found iteratively if $|\delta\beta_1(\Phi_v,\beta_0)| \approx O(\epsilon)$. We denote

$$\Phi_1(\Phi_v,\beta_v) = \Phi_{1N}(\Phi_v,\beta_v) + \Phi_{1R}(\Phi_v,\beta_v) , \tag{25}$$

where $\Phi_{1N}(\Phi_v,\beta_v)$ is the *nonsecular* solution to Eq. (10) with the resonant terms, $\delta_{M,N}$ and $\alpha_{M,N}$ neglected, and $\Phi_{1R}(\Phi_v,\beta_v)$ is the resonant contribution.

With a straightforward ordering in ϵ we define

$$\tilde{\Phi}_{1N}(\Phi_v,\beta_0) \equiv \Phi_{1N}(\Phi_v,\beta_v) , \tag{26}$$

where we iterate Eq. (24) to express β_v in terms of Φ_v and β_0 (β_0 is the label for the best calculation of a fixed field line just on the outer side of S when resonant terms are neglected). Thereby, β_v is now considered a function of β_0 and Φ_v. Note that upon splitting $\tilde{\Phi}_{1N}$ into two parts,

$$\tilde{\Phi}_{1N} = \tilde{\Phi}_{1N}^{(1)} + \tilde{\Phi}_{1N}^{(2)} , \tag{27}$$

and by defining

$$\Delta x_0(p) = \Delta x_0^{(1)}(p) + \Delta x_0^{(2)}(p) \equiv x_0(p) - x , \tag{28}$$

we obtain

$$2a\frac{\partial\tilde{\Phi}_{1N}^{(1)}}{\partial\Phi_v} = \frac{2p}{B_0^2}\delta_N(\Phi_v,\beta_0) , \tag{29}$$

$$2a\frac{\partial\tilde\Phi_{1N}^{(2)}}{\partial\Phi_v}=2a\left(\frac{x_0(p)-x}{g}+\frac{\partial\delta\beta_1}{\partial\Phi_v}\right)\frac{\partial\tilde\Phi_{1N}^{(1)}}{\partial\beta_0}-\left[\left(\frac{\partial\tilde\Phi_{1N}^{(1)}}{\partial\beta_0}+\frac{a|\nabla\alpha_v|_0^2x_c}{g}\right)^2\frac{1}{|\nabla\alpha_v|^2}\right]_N-\left(\frac{\partial\tilde\Phi_{1N}^{(1)}}{\partial\Phi_v}\right)^2+\frac{2p}{B_0^2}\delta\beta_1\frac{\partial\delta_N(\Phi_v,\beta_0)}{\partial\beta_0}+1+\frac{2p}{B_0^2}-a^2, \quad (30)$$

where

$$\tilde\Phi_{1N}^{(1)}\approx\Delta x_0^{(1)}(p)\approx O(\epsilon),\quad \tilde\Phi_{1N}^{(2)}\approx\Delta x_0^{(2)}(p)\approx O(\epsilon^2).$$

We have used the following notation for the second term on the right-hand side of Eq. (30):

$$[G(\Phi_v,\beta_0)]_N=\sum_{m,n}G_{m,n}\exp\left(\frac{i(n-mx_0(p))\Phi_v}{g}-im\beta_0\right)-G_R(M\psi),$$

$$G_R(M\psi)=\sum_r G_{rM,rN}\exp(-irM\psi),$$

where the resonance angle ψ is defined by

$$\psi=\beta_0-\left(\frac{N}{M}-x_0(p)\right)\frac{\Phi_v}{g}.$$

We also observe that we have treated $\alpha_{\max}$ as arbitrary, but we shall calculate to high enough order so that a correct expression for the rotational transform, $x_0(p)$, is obtained even when $\alpha_{\max}\approx\epsilon$.

To obtain the expressions for $\delta\beta_1$ and the nonresonant rotational transform shift $\Delta x_0(p)$, we consider the following equation:

$$\frac{d\beta_v}{d\Phi_v}=\frac{\partial H/\partial P_\beta}{\partial H/\partial P_\phi}=\frac{1}{|\nabla\alpha_v|^2}\frac{\partial\Phi(\Phi_v,\beta_v)/\partial\beta_v}{\partial\Phi(\Phi_v,\beta_v)/\partial\Phi_v}. \quad (31)$$

Upon neglecting the resonant terms on the right-hand side of Eq. (31), ordering in ϵ, and using Eq. (24), we have

$$\frac{d\beta_v}{d\Phi_v}=\frac{d\delta\beta_1}{d\Phi_v}+\frac{[x_0(p)-x]}{g}, \quad (32)$$

$$\frac{\partial\Phi(\Phi_v,\beta_v)}{\partial\Phi_v}=a+\frac{\partial\tilde\Phi_{1N}^{(1)}(\Phi_v,\beta_0)}{\partial\Phi_v}+O(\epsilon^2), \quad (33)$$

$$\frac{\partial\Phi(\Phi_v,\beta_v)}{\partial\beta_v}=\frac{\partial\tilde\Phi_{1N}^{(1)}(\Phi_v,\beta_0)}{\partial\beta_0}-\frac{\partial\delta\beta_1}{\partial\beta_0}\frac{\partial\tilde\Phi_{1N}^{(1)}(\Phi_v,\beta_0)}{\partial\beta_0}+\frac{ax_c|\nabla\alpha_v|_0^2}{g}+\frac{\partial\tilde\Phi_{1N}^{(2)}(\Phi_v,\beta_0)}{\partial\beta_0}+O(\epsilon^3). \quad (34)$$

Thus, correct to $O(\epsilon)$, we have

$$\frac{d\delta\beta_1}{d\Phi_v}=\left(\frac{1}{a|\nabla\alpha_v|^2}\frac{\partial\tilde\Phi_{1N}(\Phi_v,\beta_0)}{\partial\beta_0}\right)_N-\frac{\Delta x_0^{(1)}(p)}{g}+\left(\frac{x_c|\nabla\alpha_v|_0^2}{g|\nabla\alpha_v|^2}\right)_N, \quad (35)$$

while correct to $O(\epsilon^2)$ we have

$$\frac{d\delta\beta_1}{d\Phi_v}=\left(\frac{1}{a|\nabla\alpha_v|^2}\frac{\partial\tilde\Phi_{1N}^{(1)}}{\partial\beta_0}\right)_N-\left(\frac{1}{a|\nabla\alpha_v|^2}\frac{\partial\delta\beta_1}{\partial\beta_0}\frac{\partial\tilde\Phi_{1N}^{(1)}}{\partial\beta_0}\right)_N-\left(\frac{(\partial\tilde\Phi_{1N}^{(1)}/\partial\beta_0)(\partial\tilde\Phi_{1N}^{(1)}/\partial\Phi_v)}{(a^2|\nabla\alpha_v|^2)}\right)_N+\left[\frac{x_c|\nabla\alpha_v|_0^2}{(g|\nabla\alpha_v|^2)}\left(1-\frac{1}{a}\frac{\partial\tilde\Phi_{1N}^{(1)}}{\partial\Phi_v}\right)\right]_N-\frac{[x_0(p)-x]}{g}+\left(\frac{1}{a|\nabla\alpha_v|^2}\frac{\partial\tilde\Phi_{1N}^{(2)}}{\partial\beta_0}\right)_N, \quad (36)$$

where $x_0(p)-x$ is the total nonresonant shift in the rotational transform to $O(\epsilon^2)$.

We begin the iteration by observing that the solution of Eq. (29), with the boundary condition for single-valuedness, $\tilde\Phi_{1N}^{(1)}[\Phi_v-2\pi g,\beta_0+2\pi x_0(p)]=\tilde\Phi_{1N}^{(1)}(\Phi_v,\beta_0)$, is

$$\tilde\Phi_{1N}^{(1)}(\Phi_v,\beta_0)=\frac{-igp}{aB_0^2}\sum_{m,n}{}'\frac{\delta_{m,n}\exp(i\psi_{m,n})}{n-mx_0(p)}, \quad (37)$$

with $\psi_{m,n}=[n-mx_0(p)]\Phi_v/g-m\beta_0$. Substituting Eq. (37) into Eq. (35) allows for the solution for $\delta\beta_1$. The condition that $\delta\beta_1$ be bounded also determines $x_0^{(1)}(p)$. We find

$$\delta\beta_1=\sum_{m,n}{}'\frac{i\exp(i\psi_{m,n})}{[n-mx_0(p)]}\times\left[\frac{pg^2}{a^2B_0^2|\nabla\alpha_v|_0^2}\left(\frac{m\delta_{m,n}}{n-mx_0(p)}+\sum_{s,t}{}'\frac{s\delta_{s,t}\alpha_{m-s,n-t}}{t-sx_0(p)}\right)-x_c\alpha_{m,n}\right], \quad (38)$$

$$x_0^{(1)}(p)-x=\frac{-pg^2}{a^2B_0^2|\nabla\alpha_v|_0^2}\sum_{m,n}{}'\frac{m\delta_{m,n}\alpha^*_{m,n}}{[n-mx_0(p)]}+x_c. \quad (39)$$

Note that $x_0^{(1)}(p)-x=O(\epsilon\alpha_{\max})$. Should $\alpha_{\max}\approx O(\epsilon)$ we need to calculate $x_0(p)$ to one more order, to obtain $x_0(p)-x$ accurately.

We now substitute Eqs. (37)–(39) into Eq. (30). The condition that $\tilde\Phi_{1N}^{(2)}$ be bounded demands that the average part of the right-hand side vanishes, from which we find after some algebra that a^2 is given by

$$a^2=\frac{1}{\mu^2\lambda_0^2}=1+\frac{2p}{B_0^2}-\overline{\left(\frac{\partial\tilde\Phi_{1N}^{(1)}}{\partial\Phi_v}\right)^2}-\overline{\left[\frac{1}{|\nabla\alpha_v|^2}\left(\frac{\partial\tilde\Phi_{1N}^{(1)}}{\partial\beta_0}+\frac{ax_c|\nabla\alpha_v|_0^2}{g}\right)^2\right]_N}+O(\epsilon^3), \quad (40)$$

where μ is given in Eq. (22) and

$$\bar A=\frac{\lim_{\Phi_v\to\infty}\left[\int_{-\Phi_v}^{\Phi_v}d\Phi_v'\,A(\Phi_v',\beta_0)\right]}{2\Phi_v}$$

denotes the definition of the average of A. Now using $p_0/\lambda_0^2=p$, where p_0 is the original unnormalized pressure, we find

$$\frac{1}{\lambda_0^2} = \left\{ 1 - \overline{\left(\frac{\partial \tilde{\Phi}_{1N}^{(1)}}{\partial \Phi_v} \right)^2} \right.$$
$$\left. - \overline{\left[\frac{1}{|\nabla \alpha_v|^2} \left(\frac{\partial \tilde{\Phi}_{1N}^{(1)}}{\partial \beta_0} + a x_c \frac{|\nabla \alpha_v|_0^2}{g} \right)^2 \right]_N} \right\}$$
$$\times \frac{\mu^2}{(1 - 2p_0/B_0^2)} . \quad (41)$$

The average quantities have the specific form

$$\overline{\left(\frac{\partial \tilde{\Phi}_{1N}^{(1)}}{\partial \Phi_v} \right)^2} = \sum_{n,m} \frac{a^2 p_0^2 |\delta_{m,n}|^2}{B_0^4}, \quad (42)$$

$$\overline{\left\{ \frac{1}{|\nabla \alpha_v|^2} \left[\left(\frac{\partial \tilde{\Phi}_{1N}}{\partial \beta_0} \right) + a x_c \frac{|\nabla \alpha_v|_0^2}{g} \right]^2 \right\}_N}$$
$$= \frac{a^2 p_0^2 g^2}{B_0^4 |\nabla \alpha_v|_0^2} \sum_{n,m}{}' \left(\frac{m^2 |\delta_{m,n}|^2}{[n - m x_0(p)]^2} \right.$$
$$\left. + \sum_{s,t}{}' \frac{m s \delta_{m,n} \delta_{s,t}^* \alpha_{s-m,t-n}}{[n - m x_0(p)][t - s x_0(p)]} \right)$$
$$- \frac{2a^2 p_0}{B_0^2} x_c \sum_{m,n}{}' \frac{m \delta_{m,n} \alpha_{m,n}^*}{n - m x_0(p)} + \frac{x_c^2 a^2 |\nabla \alpha_v|_0^2}{g^2} . \quad (43)$$

We also note that in Eqs. (42) and (43), we can use the approximation $a^2 = a_0^2 = 1 + 2p/B_0^2 = 1/(1 - 2p_0/B_0^2)$ and $p = p_0/(1 - 2p_0/B_0^2)$.

To obtain $x_0(p)$ to second order, we note that in Eq. (36) the boundedness condition on $\delta\beta_1$ demands that the average of the right-hand side vanish. We observe that a tedious calculation of $\tilde{\Phi}_{1N}^{(2)}$ is needed if one is to obtain an expression correct to $O(\epsilon^2)$ to all orders to $\alpha_{\max}$. However, the average of the last term in Eq. (36) is $O(\alpha_{\max}\epsilon^2)$, whereas the average of the first term is $O(\alpha_{\max}\epsilon)$. Thus the last term is always small compared to the first term, even when $\alpha_{\max} \gtrsim \epsilon$, and we can neglect the last term in Eq. (36). Then when we set the average of the remaining terms of the right-hand side of Eq. (36) to zero, we find

$$x_0(p) = x + x_c + \sum_{n,m}{}' \frac{p_0^2 g^2}{|\nabla \alpha_v|_0^2 B_0^4} \frac{m |\delta_{m,n}|^2}{[n - m x_0(p)]}$$
$$\times \left(\frac{1}{|\nabla \alpha_v|_0^2} \frac{g^2 m^2}{[n - m x_0(p)]^2} + 1 \right)$$
$$- \frac{p_0 g^2}{B_0^2 |\nabla \alpha_v|_0^2} \sum_{n,m}{}' \frac{m \delta_{m,n} \alpha_{m,n}^*}{[n - m x_0(p)]}$$
$$+ O(\epsilon^3) + O(\epsilon^2 \alpha_{\max}) . \quad (44)$$

We now consider the equation for $\Phi_{1R}(\Phi_v, \beta_v) = \tilde{\Phi}_{1R}(\Phi_v, \beta_0)$, the resonant contribution. To leading order in $p\delta_R(M\psi)/B_0^2 \equiv \epsilon_R$ [see just after Eq. (30) for definitions] we obtain from Eq. (10) the following equation for $\tilde{\Phi}_{1R}(\Phi_v, \beta_0)$:

$$2a \left. \frac{\partial \tilde{\Phi}_{1R}}{\partial \Phi_v} \right|_{\beta_0} + \frac{1}{|\nabla \alpha_v|^2} \left[\left(\frac{\partial \tilde{\Phi}_{1R}}{\partial \beta_0} \right) \Big|_{\Phi_v} \right]^2 = \frac{2p}{B_0^2} \delta_R(M\psi) , \quad (45)$$

where we have upgraded the order of $\partial \tilde{\Phi}_{1R}/\partial \beta_0$ to be $O(\epsilon_R^{1/2})$, so that the three terms in Eq. (45) are comparable.

Let us further assume that we can treat as higher order the terms in Eq. (45) that depend on both Φ_v and ψ. Then, in Eq. (45) we approximate $1/|\nabla \alpha_v|^2$ as

$$\frac{1}{|\nabla \alpha_v|^2} = \frac{1}{|\nabla \alpha_v|_0^2} [1 + \alpha_R(M\psi)] ,$$

where

$$\alpha_R(M\psi) = \sum_r \alpha_{rM,rN} \exp(-irM\psi) .$$

This procedure can be justified using a space averaging technique that we will not attempt to formulate here.

Equation (45) now has Φ_v as an ignorable coordinate if ψ rather than the β_0 is treated as an independent coordinate. In terms of ψ and Φ_v, Eq. (45) becomes

$$2a \left. \frac{\partial \tilde{\Phi}_{1R}}{\partial \Phi_v} \right|_{\psi} - \frac{2a}{g} \left(\frac{N}{M} - x_0(p) \right) \frac{\partial \tilde{\Phi}_{1R}}{\partial \psi} + \frac{1}{|\nabla \alpha_v|_0^2} \left(\frac{\partial \tilde{\Phi}_{1R}}{\partial \psi} \right)^2$$
$$\times [1 + \alpha_R(M\psi)] = \frac{2p}{B_0^2} \delta_R(M\psi) . \quad (46)$$

Equation (46) is of Hamiltonian form with momenta $P_\psi = \partial \tilde{\Phi}_{1R}/\partial \psi$ and $\delta P_\phi = \partial \tilde{\Phi}_{1R}/\partial \Phi_v|_\psi$. Since the variable Φ_v is ignorable in this Hamiltonian, $\delta P_\phi = \partial \tilde{\Phi}_{1R}/\partial \Phi_v|_\psi = \text{const}$. Equation (46) can be separated by letting $\tilde{\Phi}_{1R} = \Phi_{1R}(\psi) + \delta P_\phi \Phi_v$, where δP_ϕ is a constant. The solution for $\partial \Phi_{1R}/\partial \psi$ is

$$g \frac{\partial}{\partial \psi} \Phi_{1R}(\psi) = a \left(\frac{N}{M} - x_0(p) \right) |\nabla \alpha_v|_0^2 [1 + \alpha_R(M\psi)]^{-1}$$
$$- a |\nabla \alpha_v|_0^2 Q(M\psi) , \quad (47)$$

where

$$Q(M\psi) = \frac{1}{[1 + \alpha_R(M\psi)]} \left[\left(\frac{N}{M} - x_0(p) \right)^2 - \frac{g^2 [1 + \alpha_R(M\psi)]}{a^2 |\nabla \alpha_v|_0^2} \left(2a \delta P_\phi - \frac{2p}{B_0^2} \delta_R(M\psi) \right) \right]^{1/2} .$$

The solution for $\tilde{\Phi}_{1R}$ is then

$$\tilde{\Phi}_{1R} = \delta P_\phi \Phi_v + \frac{a |\nabla \alpha_v|_0^2}{g} \left(\frac{N}{M} - x_0(p) \right) \int_0^\psi \frac{d\psi'}{[1 + \alpha_R(M\psi')]}$$
$$- \frac{a}{g} |\nabla \alpha_v|_0^2 \int_0^\psi d\psi' \, Q(M\psi') . \quad (48)$$

The constant δP_ϕ is determined by the condition that we do not obtain anymore toroidal current than what we have already accounted for in calculating x_c. This demands that Φ_{1R} does not change if ψ changes by $2\pi/M$ at fixed Φ_v. This leads to the condition that determines δP_ϕ:

$$\frac{N}{M} - x_0(p) = \frac{\int_0^{2\pi} d\psi \, Q(\psi)}{\int_0^{2\pi} d\psi [1 + \alpha_R(\psi)]^{-1}} . \quad (49)$$

Note from this condition that the sign of the square root in the definition $Q(M\psi)$ is the sign of $N/M - x_0(p)$.

To evaluate the change of rotational transform caused by the resonance term, we have, from Eqs. (31) and (32),

$$\frac{d\beta_v}{d\Phi_v}=\frac{1}{|\nabla\alpha_v|^2}\frac{\partial\Phi(\Phi_v,\beta_v)/\partial\beta_v}{\partial\Phi(\Phi_v,\beta_v)/\partial\Phi_v}$$
$$=\frac{1}{|\nabla\alpha_v|^2}\frac{\partial\Phi_{1N}(\Phi_v,\beta_v)/\partial\beta_v[1+O(\epsilon_R)]}{(a+\partial\Phi_{1N}/\partial\Phi_v)}$$
$$+\frac{1}{a|\nabla\alpha_v|^2}\frac{\partial\Phi_{1R}}{\partial\beta_v}[1+O(\epsilon)]\,. \qquad (50)$$

With the definition

$$\beta_v\equiv\beta_0+\delta\beta_1+[x_0(p)-x]\Phi_v/g\,, \qquad (51)$$

we have, from Eqs. (50), (51), and the definition of ψ,

$$\frac{d\beta_0}{d\Phi_v}=\frac{\partial\tilde{\Phi}_{1R}/\partial\psi}{a|\nabla\alpha_v|^2}=\frac{d}{d\Phi_v}\left[\psi+\left(\frac{N}{M}-x_0(p)\right)\frac{\Phi_v}{g}\right]. \qquad (52)$$

Therefore using Eqs. (52) and (47) and keeping only resonance terms in $|\nabla\alpha_v|^2$, we have

$$\frac{d\psi}{d\Phi_v}=-\frac{1}{g}\left(\frac{N}{M}-x_0(p)\right)+\frac{1+\alpha_R(M\psi)}{a|\nabla\alpha_v|_0^2}\frac{\partial\tilde{\Phi}_{1R}}{\partial\psi}$$
$$=-\frac{Q(M\psi)[1+\alpha_R(M\psi)]}{g}. \qquad (53)$$

We define $\Delta\Phi_v$ as the change in Φ_v when ψ changes by $2\pi/M$. Then integrating Eq. (53) over a period in ψ, gives

$$\Delta\Phi_v=-(g/M)\int_0^{2\pi}\frac{d\psi}{Q(\psi)[1+\alpha_R(\psi)]}. \qquad (54)$$

The change of the rotational transform, $\Delta x_R(p)$, caused by the resonance term, is given by

$$\Delta x_R(p)\equiv g\Delta\beta_0/\Delta\Phi_v\,, \qquad (55)$$

where $\Delta\beta_0$ is the change of β_0 when ψ changes by $2\pi/M$. Then, using

$$\Delta\beta_0=\Delta\left[\psi+\left(\frac{N}{M}-x_0(p)\right)\frac{\Phi_v}{g}\right]$$
$$=\frac{2\pi}{M}+\left(\frac{N}{M}-x_0(p)\right)\frac{\Delta\Phi_v}{g} \qquad (56)$$

and Eq. (54), we find

$$\Delta x_R(p)=\left(\frac{N}{M}-x_0(p)\right)+\frac{2\pi g}{M\Delta\Phi_v}, \qquad (57)$$

where $\Delta\Phi_v$ is given by Eq. (54).

The total change of rotational transform is

$$x(p)=x_0(p)+\Delta x_R(p)=N/M+2\pi g/M\Delta\Phi_v\,, \qquad (58)$$

where $\Delta x_0(p)$ is given by Eq. (44) and $\Delta x_R(p)$ is given by Eqs. (57) and (54).

We also note that at fixed $\beta_0+x_0(p)\Phi_v/g$, the change in $\tilde{\Phi}$ in a toroidal transit is

$$\Delta\Phi_{\rm tor}=\tilde{\Phi}[\Phi_v+2\pi g,\beta_0-2\pi x_0(p)]-\tilde{\Phi}(\Phi_v,\beta_0)$$
$$=2\pi g/[\lambda_0(p)+\delta P_\phi]\,. \qquad (59)$$

Hence

$$\frac{1}{\lambda(p)}=\frac{\Delta\Phi_{\rm tor}}{2\pi g}=\frac{1}{\lambda_0(p)}+\delta P_\phi\,. \qquad (60)$$

We now evaluate $x_0(p)$ more explicitly. First of all observe that as we change a parameter such as pressure or toroidal current, then if $Q(\psi)\to 0$ somewhere in the interval of integration, a separatrix is approached. In this case one can readily ascertain that $\Delta\Phi_v\to\infty$ logarithmically. Hence from Eq. (58) at the separatrix, $x(p)\to N/M$. Far from the separatrix, we can assume the term containing $[N/M-x_0(p)]^2$ in the square root terms of Eqs. (49) and (54) is the largest. Then expanding these two equations to linear order in δP_ϕ and quadratic order in δ_R^2, we find

$$\delta P_\phi=\frac{-p^2g^2}{2a^3B_0^4}\frac{1}{|\nabla\alpha_v|_0^2}\frac{\int_0^{2\pi}d\psi\,\delta_R^2(\psi)[1+\alpha_R(\psi)]}{2\pi[N/M-x_0(p)]^2}, \qquad (61)$$

$$\Delta\Phi_v=-\frac{2\pi g}{[N-Mx_0(p)]}\times\left(1+\frac{\delta P_\phi g^2}{a|\nabla\alpha_v|_0^2[N/M-x_0(p)]^2}-\frac{pg^2\int_0^{2\pi}d\psi\,\alpha_R(\psi)\delta_R(\psi)}{a^2|\nabla\alpha_v|_0^2[N/M-x_0(p)]^22\pi}+\frac{3g^4}{4\pi}\frac{p^2}{a^4B_0^4|\nabla\alpha_v|_0^4}\times\frac{\int_0^{2\pi}d\psi d\delta_R^2(\psi)[1+\alpha_R(\psi)]^2}{[N/M-x_0(p)]^4}\right). \qquad (62)$$

Using Eq. (61), and expanding in a Fourier expansion, we find

$$\Delta\Phi_v=-\frac{2\pi g}{[N-Mx_0(p)]}\times\left(1+\sum_r\frac{g^4p^2|\delta_{rM,rN}|^2}{a^4B_0^4|\nabla\alpha_v|_0^4[N/M-x_0(p)]^4}-\frac{g^2p\delta_{rM,rN}\alpha^*_{rM,rN}[1+O(\epsilon_R)]}{a^2\nabla\alpha_v|_0^2B_0^2[N/M-x_0(p)]^2}\right). \qquad (63)$$

Substituting Eq. (63) into Eq. (58) then yields

$$x(p)=x_0(p)+\sum_r\left(\frac{g^4p_0^2|\delta_{rM,rN}|^2}{B_0^4|\nabla\alpha_v|_0^4[N/M-x_0(p)]^3}-\frac{g^2p_0\delta_{rM,rN}\alpha^*_{rM,rN}}{|\nabla\alpha_v|_0^2B_0^2[N/M-x_0(p)]}\right). \qquad (64)$$

Similarly, from Eqs. (60) and (61), we have

$$\frac{1}{\lambda(p)}=\frac{1}{\lambda_0(p)}\left[1-\frac{p_0^2g^2}{2B_0^4|\nabla\alpha_v|_0^2}\times\sum_r\frac{1}{[N/M-x_0(p)]^2}\left(|\delta_{rM,rN}|^2+\sum_s\delta_{rM,rN}\delta^*_{sM,sN}\alpha_{(s-r)M(s-r)N}\right)\right], \qquad (65)$$

where we have used $\lambda_0(p)=1/a$. Observe that, when somewhat off-resonance, Eqs. (64) and (65) give a contribution from the resonance term that matches the most resonant contribution from the nonresonant terms given in Eqs. (44) and (40) [together with Eq. (43)], which indicates that the results of our special resonant methods overlap with the results of the nonresonant method.

It is interesting to consider in somewhat more detail the structure of our result at resonance. To do this explicitly, let us assume all $\alpha_{m,n} = 0$ and in the spectrum $\delta_{rM,rN}$, only $r = \pm 1$ terms are important. Further, we assume the $\delta_{m,n}$ are real and there is zero net equilibrium current so that $x_c = 0$. In this case Eq. (44), $Q(M\psi)$, and Eq. (48) become

$$\Delta x_0(p) = x_0(p) - x = \sum_{n,m}{}' \frac{p^2 g^2 |\delta_{m,n}|^2}{a^4 |\nabla\alpha_v|_0^2 B_0^4 [n/m - x_0(p)]} \times\left(\frac{g^2}{|\nabla\alpha_v|_0^2 [n/m - x_0(p)]^2} + 1\right), \tag{66}$$

$$Q(M\psi) = \pm\left[\left(\frac{N}{M} - x_0(p)\right)^2 - \frac{g^2}{a^2|\nabla\alpha_v|_0^2}\left(2a\delta P_\phi - \frac{4p\delta_{M,N}}{B_0^2}\cos M\psi\right)\right]^{1/2}, \tag{67}$$

where we have explicitly indicated that either the plus or minus may be the appropriate choice for $Q(M\psi)$.

$$\tilde{\Phi}_{1R} = \delta P_\phi \Phi_v + a\frac{|\nabla\alpha_v|_0^2}{g}\left(\frac{N}{M} - x_0(p)\right)\psi - \frac{a}{g}|\nabla\alpha_v|_0^2 \int_0^\psi d\psi'\, Q(M\psi'). \tag{68}$$

The condition for zero current, which is the requirement that $\tilde{\Phi}_{1R}$ be nonsecular in ψ for constant Φ_v [i.e., $\tilde{\Phi}_{1R}(\psi=0) = \tilde{\Phi}_{1R}(\psi = 2\pi/M)$], then gives

$$\frac{N}{M} - x_0(p) = \frac{1}{2\pi}\int_0^{2\pi} d\psi\, Q(\psi), \tag{69}$$

where the integral on the right-hand side can be expressed in terms of an elliptic integral if desired.

Now, let $p_{N/M}$ be a pressure that would produce a separatrix (i.e., where the total rotational transform is N/M as previously discussed). Further, we define $p^*_{N/M}$ such that $x_0(p^*_{N/M}) = N/M$. We now show that for sufficiently small $\delta_{M,N}$ there are two solutions for $p_{N/M}$, $p^+_{N/M}$, and $p^-_{N/M}$, near $p^*_{N/M}$, such that

$$p^-_{N/M} < p^*_{N/M} < p^+_{N/M}\,. \tag{70}$$

Further, in the interval

$$p^-_{N/M} < p < p^+_{N/M}\,, \tag{71}$$

there are no single-valued, zero net toroidal current solutions, while outside there intervals, if N/M is arbitrary and $\delta_{N,M}$ sufficiently small, this perturbation calculation exhibits its zero net toroidal current solutions.

To calculate $p^\pm_{N/M}$, we note that as $p^\pm_{N/M}$ represents a separatrix solution, the amplitude of the cosine term in $Q(\psi)$ is equal to the constant term. The integral in Eq. (69) is then readily evaluated and we find

$$x_0(p^\pm_{N/M}) - \frac{N}{M} = \pm 2\frac{\sqrt{2}}{\pi}\left(\frac{4g^2 p^*_{N/M}|\delta_{M,N}|}{a^2 B_0^2 |\nabla\alpha_v|_0^2}\right)^{1/2}, \tag{72}$$

$$\delta P_\phi = \frac{-2p_{N/M}}{aB_0^2}|\delta_{M,N}| + \frac{a|\nabla\alpha_{v_0}|^2}{2g^2}\left(\frac{N}{M} - x_0(p^*_{N/M})\right)^2, \tag{73}$$

where for definiteness we have assumed $x_0(p^+_{N/M}) > N/M$.

If we now expand about $p = p^*_{N/M}$, we find, using Eq. (44),

$$x_0(p^\pm_{N/M}) - \frac{N}{M} = (p^\pm_{N/M} - p^*_{N/M})\frac{dx_0(p^*_{N/M})}{dp} + \cdots = \frac{2(p^\pm_{N/M} - p^*_{N/M})\Delta x_0(p^*_{N/M})}{p^*_{N/M}}\left(1 + \sum_{n,m}{}' \frac{g^2 p^{*2}_{N/M}|\delta_{m,n}|^2\{3g^2/|\nabla\alpha_v|_0^2[n/m - x_0(p^*_{N/M})]^{-2} + 1\}}{a^4|\nabla\alpha_v|_0^2 B_0^4 [n/m - x_0(p^*_{N/M})]^2}\right)^{-1}. \tag{74}$$

For simplicity let us assume that the summation term in the denominator of Eq. (74) is much less than unity. To estimate the restriction that this assumption imposes, we further assume $N \gg 1$, $M \gg 1$, and consider those n's and m's with values $n = N + O(1)$, $m = M + O(1)$ for which $\delta_{m,n} \approx \delta_{M,N}$ and $n/m - x_0(p^*_{N/M}) = O(|M|^{-1})$. The contribution to those sums from terms in n and m can then be roughly evaluated to give the restriction

$$g^2 p^*_{N/M}|\delta_{M,N}|/|\nabla\alpha_v|_0^2 B_0^2 < 1/M^2. \tag{75}$$

The terms far from resonance in the sum of Eq. (74) add a contribution that is very roughly $O[\Delta x_0(p^*_{N/M})]$, and we need to restrict ourselves to the case $\Delta x_0(p^*_{N/M}) \ll 1$.

We now substitute Eq. (74) into Eq. (72), and we find upon iteration,

$$p^\pm_{N/M} = p^*_{N/M} \pm \frac{p^*_{N/M}\sqrt{2}}{\pi\Delta x_0(p^*_{N/M})} \times\left(\frac{4g^2 p^*_{N/M}|\delta_{M,N}|}{a^2 B_0^2 |\nabla\alpha_v|_0^2}\right)^{1/2}\left[1 + O\left(\frac{p^\pm_{N/M} - p^*_{N/M}}{p^*_{N/M}}\right)\right]. \tag{76}$$

The condition $|p^\pm_{N/M} - p^*_{N/M}|/p^*_{N/M} \ll 1$ then requires

$$\frac{g^2 p^*_{N/M}|\delta_{M,N}|}{B_0^2|\nabla\alpha_v|_0^2} \ll |\Delta x_0^2(p^*_{N/M})|\,. \tag{77}$$

We define a minor resonance at $x_0(p^*_{N/M}) = N/M$ as the condition

$$\frac{g^2 p^*_{N,M}|\delta_{M,N}|}{(B_0^2|\nabla\alpha_v|_0^2)} \ll \mathrm{Min}\left(\frac{1}{M^2}, \Delta x_0^2(p^*_{N/M})\right). \tag{78}$$

If the inequality given in Eq. (78) is satisfied, as well as $\Delta x_0(p^*_{N/M}) \ll 1$, then Eq. (76) gives the values of $p = p^\pm_{N/M}$ on the separatrix. There are no single-valued solutions in the interval given by Eq. (71) for sharp boundary equilibria with zero net toroidal current. Of course with a specified net toroidal current, one may find equilibria in the pressure interval given in Eq. (71), but the gaps in the pressure would then be shifted to other values that can be calculated using the methods developed here.

As a numerical example, let us consider the case of only two harmonic pairs, $\delta_{\pm(m,n)}$ with $|\delta_{\pm(M,N)}| \ll |\delta_{\pm(m,n)}|$. When $\delta_{M,N} = 0$ a solution can be obtained exactly in terms of elliptic integrals. With the notation $\bar{x}_0(\beta) = x_0(\beta B_0^2/2)$ and with the parameters $x = 0.245$, $g/|\nabla\alpha_v|_0 = 1$, $\delta_{3,1} = \delta_{-3,-1} = 5\times 10^{-2}$, the exact solution to $x_0(\beta^*_{1/4}) = 0.25$ is $\beta^*_{1/4}$ (exact) $= 0.05210$, where $\beta^*_{1/4} = 2p^*_{1/4}/B_0^2$.

The approximate solution for $\bar{x}_0(\beta^*_{1/4})$ using Eq. (66) becomes

$$\bar{x}_0(\beta^*_{1/4}) = x + \frac{\beta^{*2}_{1/4}}{2a^4}|\delta_{3,1}|^2 \frac{1 + [\frac{1}{3} - x_0(\beta^*_{1/4})]^2}{[\frac{1}{3} - x_0(\beta^*_{1/4})]^3}.$$

Thus, replacing $\bar{x}_0(\beta^*_{1/4})$ by 0.25, we can get the value for $\beta^*_{1/4} \equiv \beta^*_{1/4}(\text{apprx}) = 0.04795a^2$ and from $a^2 = 1 + \beta$, we obtain $\beta^*_{1/4}(\text{apprx}) = 0.05036$. The error is $e = [\beta^*_{1/4}(\text{apprx}) - \beta^*_{1/4}(\text{exact})]/\beta^*_{1/4}(\text{exact}) = 3.3\times 10^{-2}$. When we include the resonant term, $\delta_{4,1} = \delta_{-4,-1} = 5\times 10^{-6}$, the equations for the gap boundaries are

$$\bar{x}_0(\beta^{\pm}_{1/4}) = \frac{1}{4} \pm \frac{4}{\pi}\left(\frac{\beta^*_{1/4}}{a^2}|\delta_{4,1}|\right)^{1/2}.$$

The solutions for $\beta^{\pm}_{1/4}$ are then found to be

$$\beta^{+}_{1/4} = 0.05300, \quad \beta^{-}_{1/4} = 0.04759.$$

Naturally, the gap defined by $\beta^{\pm}_{1/4}$ is centered around $\beta^*_{1/4}$ (exact). If we shift the gap by the amount $\beta^*_{1/4}$(exact) $- \beta^*_{1/4}$(apprx), we obtain the corrected values

$$\beta^{+}_{1/4}(\text{corrected}) = 0.05474,$$

$$\beta^{-}_{1/4}(\text{corrected}) = 0.04933.$$

Figure 1 shows the results of the numerical solution of Eq. (12). The dashed line is the rotational transform with only one harmonic pair, $\delta_{\pm(3,1)} = 0.05$. The result is known exactly, so that no iteration is involved. The dots show the rotational transform when $\delta_{4,1} = 5\times 10^{-6}$ is added to the $\delta_{m,n}$ spectrum. The solutions are obtained by looking for zero current by iteration, and the error bars denote the uncertainty in the value of the rotational transform when the field line is followed for a finite interval. The corrected values $\beta^{\pm}_{1/4}$ are plotted as vertical lines. It can be readily seen that excellent agreement is obtained between the numerical results and the analytic predictions for the gap. No equilibria are found in the beta gap and the size of the gap correlates well with the analytic calculation.

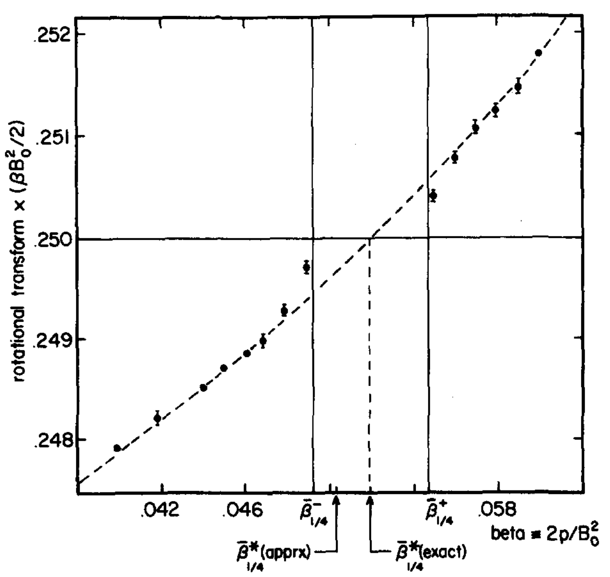

FIG. 1. Structure of the gap in beta for zero net toroidal current equilibria. The parameters chosen are $\alpha_{m,n} = 0$, $\delta_{n,m} = 0$ except for $\delta_{3,1} = \delta_{-3,-1} = 5\times 10^{-2}$, $\delta_{4,1} = \delta_{-4,-1} = 5\times 10^{-6}$, and $g/|\nabla\alpha_v|_0 = 1$. The dashed curve is the exact solution for $x_0(\beta B_0^2/2)$ and the large dots are the numerical solution obtained by integrating the solutions of the equations for the characteristics with those initial values that produce zero toroidal current.

We conclude with a brief discussion of ergodic structure. It is well known in Hamiltonian dynamics problems[14] that near the separatrix, the solutions in a surface of section plot will be ergodic in an exponentially small interval of energy near the separatrix. Thus we observe that in our problem near the separatrix the magnetic field will be ergodic in an exponentially small interval of pressure even if the inequality Eq. (78) is valid. As the inequality becomes less well satisfied, the ergodic interval increases. Roughly, the breakdown of Eq. (78) is equivalent to the island overlap condition, for which our technique of isolating a single resonance term is totally invalid. To treat the ergodic solutions in more detail requires additional techniques that we will not develop here. However, many properties of the ergodic behavior can be determined from known results.[14]

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APPENDIX: COMMENTS ON ASSUMPTIONS AND OTHER TOPICS

A fundamental assumption of this paper is that there are systems without symmetry where an exact vacuum field magnetic flux surface with irrational rotational transform exists. As mentioned in the text, this assumption can be proved rigorously for systems whose deviation from symmetry can be treated as a perturbation. Given a parameter ϵ that measures the deviation from symmetry, KAM analysis establishes a lower bound on the value of ϵ where one finds flux surfaces. It is expected, and we have assumed, that one will be able to find surfaces even for $\epsilon \gtrsim 1$ (fully three-dimensional equilibria). This statement is suggested from Greene's analysis of the standard map for the determination of the breakdown of the last KAM surface,[17] modern renormalization theory in nonlinear dynamics,[14] and many direct numerical calculations of vacuum magnetic flux surfaces in three-dimensional configurations.[18,19]

In regard to finding vacuum flux surfaces, it is of interest to consider the following problem. Suppose we are given a toroidal surface S enclosing a zero current region and we wish to determine if this surface can be a vacuum flux surface. We observe that the following Neumann problem has a unique solution: find $\Phi_v(\mathbf{r})$ inside S given that $\nabla^2\Phi_v(\mathbf{r}) = 0$

inside S, $\partial\Phi_v/\partial n = 0$ on S, and that Φ_v changes by unity along any path that returns to its point of origin after one toroidal circuit and an arbitrary number of poloidal circuits.

The solution to this problem is unique. It follows that the magnetic field ($\mathbf{B}_v = \nabla\Phi_v$) on S either generates a magnetic flux surface with an irrational rotational transform, or the magnetic field closes on itself.

An interesting question that we have not solved is to determine, given the surface S, some general statements as to when a flux surface exists (i.e., where one magnetic field line generates the entire surface). For certain classes of surfaces with near helical symmetry, flux surfaces should be generated nearly always. However, it is possible that if the surface is too far away from any symmetry, one will find that the field lines generated on S all close on themselves. Such a situation is reminiscent of results with circle maps where with a large enough perturbation, one cannot find curves with irrational winding numbers, just rational curves.[20]

One special degenerate case is a surface S that is toroidally symmetric. The solution to this problem is

$$\Phi_v = \phi/2\pi ,$$

where ϕ is the conventional azimuthal angle about the axis of symmetry $\hat{\mathbf{z}}$. Clearly, the magnetic field lines lie on S but close on themselves and the rotational transform is zero.

We can still attempt to find a sharp boundary equilibrium on the surface S and seek single-valued solutions for P_ϕ and P_β of Eq. (12) with a pressure p_0 inside the surface S. If we demand that the toroidal plasma current is zero, there are no solutions, as it is well known that zero toroidal current stellarators do not exist with toroidal symmetry. However, if we allow solutions with finite toroidal current on the surface S, then solutions exist. We are then describing a sharp boundary tokamak. There of course remains the important physical problem of determining the vacuum currents that one must add in vacuum vertical field coils outside S to support the plasma contained within the surface S. This problem has a well-defined answer.

We showed in the text that given S, gaps occur as one varies p_0 and the total plasma toroidal current. In these gaps one cannot find solutions. When one considers a surface with toroidal symmetry, the gap always encompasses the region of zero toroidal current.

We conclude with the following brief discussion. In developing our Hamiltonian formalism we chose to use Φ_v and β_v as independent coordinates. This choice may be somewhat confusing because β_v is not a usual surface coordinate in that the condition for single-valuedness of a function $G(\Phi_v,\beta_v)$ is

$$G(\Phi_v + 2\pi g,\beta_v - 2\pi x) = G(\Phi_v,\beta_v) .$$

If, instead, one uses Φ_v and θ [defined by Eq. (3)] as coordinates, the single-valuedness condition for a function $\tilde{G}(\Phi_v,\theta)$ has the usual form

$$\tilde{G}(\Phi_v + 2\pi g,\theta) = \tilde{G}(\Phi_v,\theta) .$$

In terms of Φ_v and θ, the Hamiltonian for the system can be written as

$$\begin{aligned} 1 + 2p_0/B_0^2 &= 2H'(\Phi_v,\theta) \\ &= \frac{1}{2}(P'_\phi + xP'_\theta)^2 + \frac{P'^2_\theta}{2|\nabla\alpha_v|_0^2} \\ &\quad \times [1 + \alpha'(\Phi_v,\theta)] - \frac{p_0}{B_0^2}\delta'(\Phi_v,\theta) , \end{aligned}$$

where

$$\delta'(\Phi_v,\theta) = \sum_{m,n} \delta_{m,n} \exp(in\Phi_v/g - im\theta) ,$$

$$\alpha'(\Phi_v,\theta) = \sum_{m,n} \alpha_{m,n} \exp(in\Phi_v/g - im\theta) ,$$

and one can readily show that $P'_\theta = P_\beta$ and $P'_\phi = P_\phi - xP_\beta$.

The arguments used in the text to reduce the Hamiltonian to one that to lowest order is a function only of momenta, will follow with nearly identical manipulations.

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