Three-dimensional plasma equilibrium near a separatrix

A. H. Reiman and N. Pomphrey
Plasma Physics Laboratory, Princeton University, Princeton, New Jersey 08543

A. H. Boozer
Department of Physics, College of William and Mary, Williamsburg, Virginia 23185

(Received 16 June 1988; accepted 30 November 1988)

The limiting behavior of a general three-dimensional magnetohydrodynamic (MHD) equilibrium near a separatrix is calculated explicitly. No expansions in beta or assumptions about island widths are made. Implications of the results for the numerical calculation of such equilibria are discussed, as well as for issues concerning the existence of three-dimensional MHD equilibria.

I. INTRODUCTION

The presence of closed magnetic field lines poses difficulties for the computation of three-dimensional magnetohydrodynamic (MHD) equilibria,[1] and even raises questions about the existence of such equilibria.[2–4] On rational magnetic surfaces (i.e., surfaces having a rational value of the rotational transform) every field line closes on itself. This leads to an apparent singularity in the pressure-driven current at such a surface. In a more realistic treatment of three-dimensional fields, the rational surfaces break up to form islands. Questions about the nature of the equilibrium solution near a rational surface are replaced by questions about the behavior in the neighborhood of a separatrix. The rotational transform becomes rational there, and the x lines are closed magnetic field lines. In this paper we calculate explicitly the limiting behavior of a general three-dimensional MHD equilibrium solution as it approaches a separatrix. Our analysis assumes a nonzero toroidal field at the separatrix. In light of our solution, we examine some of the issues concerning the existence of three-dimensional MHD equilibria. We also discuss some implications for the numerical computation of such equilibria.

Magnetohydrodynamic equilibria near a separatrix have been calculated analytically for a simple model field,[5] and for narrow islands at low beta.[6,7] The analysis of this paper is based on the observation that the behavior of the MHD equilibrium near a separatrix is dominated by the X point, so that considerable information about the leading-order behavior can be extracted quite generally, without making any assumptions about island width or beta.

The plasma equilibrium equation, assuming a scalar pressure, is

$$\mathbf{j}\times\mathbf{B}=\nabla p, \tag{1}$$

with

$$\nabla\times\mathbf{B}=\mathbf{j}. \tag{2}$$

In the absence of a pressure gradient, the equilibrium equation implies only that the current density is aligned with the magnetic field. No particular difficulties arise at closed magnetic field lines. Adding a finite pressure gradient produces a component of the current density perpendicular to the magnetic field,

$$\mathbf{j}_\perp=\mathbf{B}\cdot\nabla p/B^2. \tag{3}$$

The component of the current density parallel to $\mathbf{B}$ must now adjust itself to satisfy the constraint that the total current density is divergence-free. That is not possible on a rational magnetic surface unless $\oint dl/B$ is constant on the surface, where the integral is evaluated along the closed field lines. This condition is generally not satisfied except in the presence of a symmetry such as axisymmetry. If $\oint dl/B$ is not constant on a rational surface, and if ∇p does not vanish, the magnitude of the parallel current density that must be added to make the total current divergence-free becomes infinitely large as the rational surface is approached.

In a more realistic treatment of three-dimensional magnetic fields, the rational surfaces are replaced by chains of magnetic islands. We will see that the singular nature of the equilibrium solutions does not persist in the neighborhood of the separatrices. A finite pressure gradient at the separatrix does not give a singular current.

Figure 1 is a sketch of the neighborhood of the x line. (The x line intersects the plane of the picture at only one point, so it is, of course, represented as an X point.) The immediate neighborhood of the separatrix is stochastic, and therefore has a flat pressure profile. Outside this narrow stochastic layer is the region of interest, which has good flux surfaces, and is therefore capable of supporting a pressure gradient.

We will use magnetic coordinates to solve for the pressure-driven current near the separatrix. In Sec. II we calculate the magnetic coordinates in the neighborhood of the x line by an expansion about the x line. The q profile is calculated in Sec. III. The calculation of the pressure-driven current is completed in Sec. IV. In Sec. V we calculate the self-

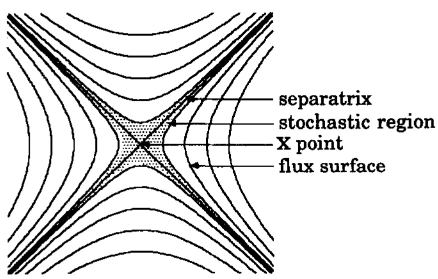

FIG. 1. Magnetic geometry in the neighborhood of an X point.

 0899-8221/89/030555-08$01.90

consistent constraint that comes out of Ampère's law. Finally, the significance of the results is discussed in Sec. VI.

Several appendices provide additional detail and consider the solutions in particular limits. Appendix A provides some details of the algebra involved in the calculation of the Θ magnetic coordinate near the x line. In Appendix B we verify that we recover the proper expression for the magnetic coordinates near a narrow island. In Appendix C, we use the Grad–Shafranov equation to give an alternative derivation of the constraint due to Ampère's law for helical and cylindrical systems. Appendix D gives expressions for the metric elements of the helical–hyperbolic coordinate system adopted in Sec. II.

II. MAGNETIC COORDINATES NEAR AN x LINE

In Sec. IV it will be seen that the equations determining the pressure-driven current simplify greatly in magnetic coordinates. In this section we obtain the solution for the magnetic coordinates near the x line. The key to our analytic solution for the magnetic coordinates in the neighborhood of the x line is a transformation to a helical–hyperbolic coordinate system, in which the equations determining the magnetic coordinates simplify.

The neighborhood of the x line is shown in Fig. 1. The x line closes on itself after traversing the torus M times in the toroidal direction and N times in the poloidal direction. (This is the case, for example, if there is an island due to a resonant perturbation having poloidal mode number M and toroidal mode number N.) The trajectory of the x line may be represented in cylindrical coordinates (R, ϕ, Z) as

$$R = R_x(\phi), \quad Z = Z_x(\phi).$$

We normalize ϕ to go from 0 to 2π in M toroidal circuits. This preserves the single-valuedness of R_x and Z_x, and it will be a convenient normalization when we Fourier decompose in the ϕ direction.

In the region of good flux surfaces, the magnetic field can be written in the form[8,9]

$$\mathbf{B} = \nabla\Psi_t \times \nabla\Theta + \nabla\Phi \times \nabla\Psi, \tag{4}$$

where Θ and Φ are poloidal and toroidal angles, respectively, and Ψ_t is a function only of Ψ. A set of coordinates (Ψ, Θ, Φ) in which the magnetic field assumes this canonical form is called "magnetic coordinates." The flux surface label Ψ_t corresponds to the toroidal flux enclosed by that surface divided by 2π. Similarly, $2\pi\Psi$ corresponds to the flux through a ribbon that coincides with a fixed value of Θ and which is bounded on one edge by the magnetic axis and on the other edge by the corresponding flux surface. Equation (4) does not uniquely specify the angles. One of the angles can be specified for our convenience. We take Φ to coincide with the cylindrical coordinate ϕ, with ϕ normalized as above.

Even after specifying $\Phi = \phi$, Θ is not uniquely determined by Eq. (4). The form of the equation is preserved by a transformation to

$$\bar{\Theta} = \Theta + (j/M)\phi,$$
$$\bar{\Psi} = \Psi + (j/M)\Psi_t,$$

where j is an arbitrary integer. The coefficient of the term linear in ϕ has been chosen to preserve the single-valuedness of Θ in the toroidal direction. (Increasing ϕ by $2M\pi$ increases $\bar{\Theta}$ by $2j\pi$.) In the following it will be assumed that Ψ is analytic in the neighborhood of the x line. We will see that Ψ is then uniquely determined by Eq. (4), as is Θ. Our Θ will wind around the torus at the same average rate as the x line, corresponding to what is often called a "helical coordinate system." We will therefore denote Ψ from now on with a subscript h, corresponding to the helical flux Ψ_h.

To understand the analyticity properties of the flux functions in the neighborhood of the x line, consider the flux through an arbitrary ribbon extending from the magnetic axis to the separatrix. If the outer edge of the ribbon winds around the magnetic axis at a rate different from that of the x line, it must intersect and cross the x line, and must have corners at those intersections. On the other hand, if the edge of the ribbon winds around with the same average pitch as that of the x line it can avoid crossing the x line, and is then smooth. The flux through this ribbon is the helical flux. This argument shows why it is reasonable that our requirement that Ψ be analytic will uniquely specify $\Psi = \Psi_h$.

Assuming that Ψ_h is an analytic function of position, its expansion about the x line takes the form

$$\begin{aligned}\Psi_h \approx {} & \Psi_{hRR}(\phi)(R - R_x)^2/2 \\ & + \Psi_{hRZ}(\phi)(R - R_x)(Z - Z_x) \\ & + \Psi_{hZZ}(Z - Z_x)^2/2,\end{aligned} \tag{5}$$

where the intersection of two flux surfaces at the x line implies that terms linear in $R - R_x$ and $Z - Z_x$ vanish, and where the value of Ψ_h on the x line can be taken to be zero without affecting the magnetic field. We apply a series of coordinate transformations that put us in a helical–hyperbolic coordinate system and simplify this expression. First, we shift our coordinate axis in the R-Z plane to the x line and transform away the cross term in the Taylor expansion by a rotation of the coordinates in the R-Z plane. Thus

$$\Psi_h = \xi^2/a^2 - \eta^2/c^2, \tag{6}$$

where a and c are functions of ϕ, and

$$\begin{aligned}R &= \xi\cos(\gamma) + \eta\sin(\gamma) + R_x, \\ Z &= \eta\cos(\gamma) - \xi\sin(\gamma) + Z_x.\end{aligned} \tag{7}$$

In these expressions $\gamma(\phi)$ is an angle determined by the second derivatives of Ψ_h at the x line, and the coefficients $a(\phi)$ and $c(\phi)$ are similarly determined by these derivatives.

Finally, we apply a transformation to hyperbolic coordinates,

$$\xi = a\rho\cosh(\alpha), \quad \eta = c\rho\sinh(\alpha), \tag{8}$$

so that Ψ_h assumes the simple form

$$\Psi_h = \rho^2. \tag{9}$$

To leading order, the surfaces of constant ρ coincide with the flux surfaces.

From Eqs. (6) and (7), it is seen that a and c are determined up to a multiplicative constant by the shape of the flux surfaces. The multiplicative constant is determined by the magnetic field through Eq. (4). Having assumed that Ψ_h is an analytic function in the neighborhood of the X point, we have been led to a unique specification of Ψ_h in terms of $\mathbf{B}$. We will later see that Ψ_h corresponds to the helical flux.

We use Eqs. (4) and (9) to evaluate B^ϕ and B^Θ in the (ρ,α,ϕ) coordinate system. This gives two partial differential equations, which together determine the magnetic coordinate Θ. The details of this calculation are given in Appendix A. The solution is

$$\Theta = \frac{1}{q_h}\left(\phi + \frac{1}{2}\int_0^\phi acRB^\alpha\,d\phi' - \frac{1}{2}acB_0\alpha\right), \qquad (10)$$

where $q_h \equiv d\Psi_t/d\Psi_h$ is the safety factor, and where we write $R\,\mathbf{B}\cdot\nabla\phi = B_0(\phi)$ to lowest order near the x line.

The multivalued piece of Θ must satisfy the condition that Θ changes by a multiple of 2π when ϕ increases by 2π. This gives a constraint on $B^\alpha(\phi)$:

$$\int_0^{2\pi} acRB^\alpha\,d\phi = 4\pi(q_h\,l - 1),$$

for some integer l. Since the left-hand side is independent of ρ, l must be zero. (In the next section it will be seen that q_h is a logarithmically singular function of ρ in the neighborhood of the separatrix.) The constraint reduces to

$$\int_0^{2\pi} acRB^\alpha\,d\phi = -4\pi. \qquad (11)$$

For the special cases of axisymmetry or helical symmetry, the integrand is independent of ϕ and we obtain an expression for B_0^α,

$$B_0^\alpha = -2/(acR). \qquad (12)$$

In Appendix B we verify that our solution for the magnetic coordinate Θ corresponds to the known solution in the narrow island limit.

We will see in the next section that $q_h \to \infty$ as we approach the separatrix, and that α can be of the same order as q_h. It follows that the term containing α dominates in Eq. (10).

III. DETERMINATION OF q

To deduce q_h from our expression for Θ we need only impose the condition that Θ goes from 0 to 2π in one poloidal circuit on any flux surface. This may seem surprising since q_h is a global characteristic of a flux surface, while the expansion of the previous section was valid only in the neighborhood of the x line. Near the separatrix, however, almost all the variation in Θ is occurring near the x line.

We express Θ in terms of ξ and Ψ_h. To do that, α is first expressed in terms of ξ and η,

$$\alpha = \tanh^{-1}(\eta a/\xi c) = \tfrac{1}{2}\ln[(\xi c + \eta a)/(\xi c - \eta a)],$$

where it has been assumed (without loss of generality) that we are working in a quadrant where $\Psi_h > 0$. For determining the boundary condition on Θ, we are interested in the limit where $\xi^2/a^2 \gg \Psi_h$ and $\eta^2/c^2 \gg \Psi_h$. We use Eq. (6) to eliminate ξ in terms of η and Ψ_h, and retain only the leading-order term in this limit,

$$\alpha \approx \pm \ln(2\xi/a\sqrt{\Psi_h}). \qquad (13)$$

For a fixed ϕ, the change in Θ in going from $-\xi$ to ξ is

$$\Delta\Theta = (acB_0/q)\ln(2\xi/a\sqrt{\Psi_h}).$$

This expression shows that in the limit, as we approach the separatrix, nearly all the variation of Θ occurs near the x line.

The intersection of any flux surface with a fixed ϕ plane defines a closed loop. Following the loop around once defines a single poloidal transit on that flux surface. The normalization of the expression for Θ must take into account the fact that in one poloidal transit on a fixed flux surface near the separatrix the same x line may be encountered more than once. The x line intersects the fixed ϕ plane in a finite set of X points. We let n_x denote the number of those X points that we pass near in one poloidal transit. If the flux surface does not enclose the magnetic axis (the surface is in the magnetic island), the x line is encountered twice ($n_x = 2$). If the flux surface does enclose the magnetic axis, $n_x = N$ (where N was defined at the beginning of Sec. II). We do not consider here the degenerate case where several independent x lines lie on the same separatrix.

The total change in Θ in one poloidal transit, to leading order in the distance from the separatrix, is

$$\Delta\Theta = (n_x B_0 ac/q)\ln(1/\sqrt{\Psi_h}). \qquad (14)$$

Requiring that this total change in Θ be equal to 2π, we determine the limiting behavior of q_h for small Ψ_h,

$$q_h = (n_x B_0 ac/\pi)\ln(1/\sqrt{\Psi_h}). \qquad (15)$$

Having Taylor expanded Ψ_h near the x line, we have obtained unique, explicit expressions for Θ near the x line and for q_h near the separatrix. From the fact that $q_h \to \infty$ as we approach the separatrix, it is clear that we are in a helical coordinate system, as claimed in the previous section.

In Appendix B we verify that our solution for q_h corresponds to the known solution in the narrow island limit.

IV. THE CURRENT

In this section we calculate the current in the neighborhood of the separatrix.

Equations (1) and (2) imply that the current is divergence-free and satisfies $\mathbf{j}\cdot\nabla\Psi_h = 0$. It follows that $\mathbf{j}$ can be written in magnetic coordinates in the form

$$\mathbf{j} = \left(I'(\Psi_h) - \frac{\partial\nu}{\partial\Theta}\right)\nabla\Psi_h\times\nabla\Theta + \left(\frac{\partial\nu}{\partial\phi} - g'(\Psi_h)\right)\nabla\phi\times\nabla\Psi_h. \qquad (16)$$

Here ν is a periodic function of Θ and ϕ, while $I'(\Psi_h) = dI/d\Psi_h$ and $g'(\Psi_h) = dg/d\Psi_h$ are the profiles of the net toroidal and poloidal current, respectively. Substituting Eq. (16) into Eq. (1) gives a magnetic differential equation which determines ν,

$$\mathbf{B}\cdot\nabla\nu = p' + g'\mathbf{B}\cdot\nabla\phi + I'\mathbf{B}\cdot\nabla\Theta, \qquad (17)$$

where $p'(\Psi_h) = dp/d\Psi_h$.

Equations (16) and (17) hold in any flux-coordinate system, that is, in any coordinate system in which the radial coordinate labels the flux surfaces. In a general coordinate system of this type, the representation of the magnetic field is similar to that of expression (4), except that terms analogous to those containing ν in Eq. (16) must be added. In a magnetic coordinate system the field lines are straight ($\mathbf{B}\cdot\nabla\Phi/\mathbf{B}\cdot\nabla\Theta$ is a function only of Ψ_h). As a consequence, derivatives along the field lines assume a simple form,

$$\mathbf{B}\cdot\nabla=\mathscr{J}^{-1}\left(\frac{\partial}{\partial\Theta}+q_h\frac{\partial}{\partial\Phi}\right),$$

where

$$\mathscr{J}^{-1}=\frac{\partial(\Psi_h,\Theta,\phi)}{\partial(x,y,z)}=\nabla\Psi_h\times\nabla\Theta\cdot\nabla\phi=B\cdot\nabla\Theta \quad (18)$$

is the Jacobian of the transformation from magnetic coordinates to Cartesian coordinates. Fourier decomposition in a magnetic coordinate system reduces magnetic differential equations to trivially soluble algebraic equations. Writing

$$\mathscr{J}(\Psi_h,\Theta,\phi)=\sum_{n,m}\mathscr{J}_{n,m}\,e^{-i(n\phi-m\Theta)} \quad (19)$$

allows the solution to Eq. (17) to be expressed in terms of the Fourier components of the Jacobian,

$$v=\frac{dp}{d\Psi_h}\sum_{n,m}{}'\frac{i\mathscr{J}_{n,m}}{(nq_h-m)}e^{-i(n\phi-m\Theta)}, \quad (20)$$

where the prime indicates that the $m=n=0$ term is omitted. The $n=m=0$ component of Eq. (17) gives a relation between g', I', and p',

$$p'\mathscr{J}_{0,0}+g'q_h+I'=0. \quad (21)$$

Equation (21) is an averaged equilibrium equation on the flux surface.

Equations (16) and (20) determine the equilibrium current, once the magnetic coordinates have been found. Since q_h appears in the denominator of Eq. (20), there is no problem as we approach the separatrix.

It follows from $q_h\to\infty$ as we approach the separatrix that the $n\neq0$ terms in the solution for v, Eq. (20), become small there. The ϕ derivative of v is therefore negligibly small relative to the Θ derivative. Retaining only the $n=0$ terms in Eq. (20), the m's cancel in the Θ derivative, giving

$$\frac{\partial v}{\partial\Theta}=p'(\Psi_h)[\mathscr{J}_{n=0}(\Theta)-\mathscr{J}_{0,0}], \quad (22)$$

where

$$\mathscr{J}_{n=0}(\Psi_h,\Theta)=\sum_m\mathscr{J}_{0,m}\,e^{im\Theta} \quad (23)$$

is the average of the Jacobian over ϕ at fixed values of Θ and Ψ_h.

Figure 2 is a sketch of the behavior of $\mathscr{J}_{n=0}$ as a function of the magnetic coordinate Θ for $n_x=1$. (We first focus on $n_x=1$, and then generalize to arbitrary n_x.) On flux surfaces near the separatrix Θ varies very rapidly near the x line, while $\mathscr{J}$ displays no such singular behavior. It follows that if we express $\mathscr{J}_{n=0}$ as a function of Θ, almost all of the variation occurs in the neighborhood of $\Theta=\pi$ (for $n_x=1$), giving the general form shown in Fig. 2. The dashed vertical line indicates the domain of validity of our expansion around the x line. (The expansion is valid to the left of the dashed line.) Our expansion is valid for $\xi/r_0<\epsilon\ll1$, where r_0 measures the poloidal scale length of the flux surface and ϵ is a small number. Letting $\Theta=\pi-\delta\Theta$, we find from Eqs. (A4), (A6), and (13) that this holds for

$$\delta\Theta>\frac{\pi}{2}\frac{\ln\epsilon}{\ln(1/\sqrt{\Psi_h})}.$$

Near the separatrix, $\mathscr{J}_{0,0}=\int_0^{2\pi}\mathscr{J}_{n=0}\,d\Theta$ is well approximated by $2\pi\mathscr{J}_{n=0}$ $(\Theta=0)$, that is, by the value of $\mathscr{J}_{n=0}$ on the x line. Recall that $\mathscr{J}=q_h/\mathbf{B}\cdot\nabla\phi$. We therefore have

$$\mathscr{J}_{0,0}=\frac{q_h(\Psi_h)}{2\pi}\int_0^{2\pi}\frac{R_x(\phi)}{B_0(\phi)}d\phi. \quad (24)$$

For $n_x>1$, the average over Θ is again dominated by the x line. Equation (24) still holds.

Near the separatrix, the current density is given by

$$\mathbf{j}=\{I'(\Psi_h)-p'(\Psi_h)[\mathscr{J}_{n=0}(\Theta)-\mathscr{J}_{0,0}]\}\nabla\Psi_h\times\nabla\Theta-g'(\Psi_h)\nabla\phi\times\nabla\Psi_h. \quad (25)$$

The fact that $\nabla\Psi_h$ is nonvanishing away from the x line implies that $p'(\Psi_h)$ cannot go to infinity at the separatrix, so the pressure-driven current remains finite there. The pressure-driven current vanishes on the x line, but may be finite elsewhere on the separatrix. This is consistent with the results of Ref. 5.

V. AMPÈRE'S LAW

In this section we complete our description of the equilibrium in the neighborhood of the separatrix by using Ampère's law to obtain a self-consistent relation between the parameters in our equilibrium solution. To motivate the work of this section, consider first the cylindrically symmetric case, where all the parameters are independent of ϕ. The poloidal components of Ampère's law involve derivatives of B^ϕ with respect to R and Z (the Cartesian coordinates in the poloidal plane). These derivatives are not determined by the lowest-order piece of B^ϕ, which is a constant. The poloidal components of Ampère's law therefore serve only to determine the next higher-order piece of B^ϕ. The ϕ component of Ampère's law for the cylindrically symmetric case, on the other hand, gives a relation between the derivatives of the poloidal components of the magnetic field and the current at the x line. This is the relation that we seek. For a cylindrically symmetric separatrix in a vacuum field, for example, it gives the well-known constraint that the separatrix comes into the X point at right angles ($a=c$). Similarly, for the helically symmetric case, the component of Ampère's law along the helix gives a constraint on the equilibrium solution near an x line. (The helical case is solved in Appendix C.) For the general case, we find that the covariant ϕ component of Ampère's law gives such a constraint.

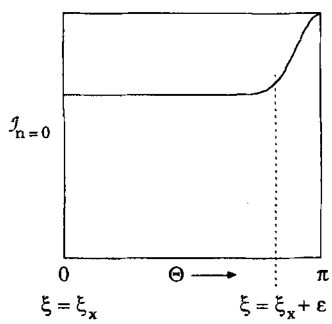

FIG. 2. A sketch of the behavior of $\mathscr{J}_{n=0}$ as a function of Θ for $n_x=1$. Almost all of the variation occurs in the neighborhood of $\Theta=\pi$.

The curl of **B** in our (ρ,α,ϕ) coordinate system is

$$J^i = (\nabla\times\mathbf{B})^i = \epsilon^{ijk}\,\partial_j(g_{kl}B^l), \tag{26}$$

where ϵ^{ijk} is the antisymmetric permutation tensor, with $\epsilon^{\rho\alpha\phi} = 1/\mathscr{J}^\rho$, and where ∂_j is the partial derivative with respect to the j coordinate. The covariant metric tensor is

$$g_{ij} = \partial_i\mathbf{x}\cdot\partial_j\mathbf{x}. \tag{27}$$

The metric elements are evaluated using Eqs. (7) and (8) and are given in Appendix D.

The evaluation of the lowest-order piece of each of the components of Eq. (26) individually requires the evaluation of ρ and α derivatives of the order ρ piece of B^ϕ. If we form

$$J_\phi = g_{\phi i}J^i, \tag{28}$$

the coefficients of the order ρ terms of B^ϕ cancel, and we are left with an expression which, to lowest order, involves only the lowest-order pieces of the magnetic field. To carry out this computation it is convenient to first express the metric elements in a form that explicitly displays that ρ dependence,

$$g_{ij} = g_{ij}^{(0)} + \rho g_{ij}^{(1)} + \rho^2 g_{ij}^{(2)}.$$

Substituting this form into Eqs. (26) and (28), we can directly evaluate the ρ derivatives and determine the lowest-order term in ρ,

$$\begin{aligned}\mathscr{J}^\rho J_\phi = \rho B^\phi\Big(&2g_{\phi\phi}^{(0)}g_{\alpha\phi}^{(1)} \\ &- g_{\phi\phi}^{(0)}\frac{\partial}{\partial\alpha}g_{\rho\phi}^{(1)} + g_{\phi\rho}^{(0)}\frac{\partial}{\partial\alpha}g_{\phi\phi}^{(1)} \\ &- g_{\phi\rho}^{(0)}\frac{\partial}{\partial\phi}g_{\alpha\phi}^{(1)} + g_{\alpha\phi}^{(1)}\frac{\partial}{\partial\phi}g_{\rho\phi}^{(0)} - g_{\alpha\phi}^{(1)}g_{\phi\phi}^{(1)}\Big) \\ &+ \rho B^\alpha\Big(2g_{\phi\phi}^{(0)}g_{\alpha\alpha}^{(2)} - g_{\phi\phi}^{(0)}\frac{\partial}{\partial\alpha}g_{\rho\alpha}^{(1)} \\ &+ g_{\phi\rho}^{(0)}\frac{\partial}{\partial\alpha}g_{\alpha\phi}^{(1)} - (g_{\alpha\phi}^{(1)})^2\Big).\end{aligned} \tag{29}$$

In this expression terms that are known to be zero from our evaluation of the metric elements have been neglected.

Finally, we substitute our explicit expressions for the metric elements into Eq. (29) to obtain the desired relation. A large amount of algebra is involved, for which we have used MACSYMA.[10] There are many cancellations. The final result is

$$\begin{aligned}\mathscr{J}^\rho J_\phi = \big[&\tfrac{1}{2}(c^2-a^2)(2R_x^2+\dot R_x^2+\dot Z_x^2) \\ &+\tfrac{1}{2}(a^2+c^2)(\dot R_x^2-\dot Z_x^2)\cos(2\gamma) \\ &-(a^2+c^2)\dot R_x\dot Z_x\sin(2\gamma)\big]B^\alpha \\ &+\{ac[\ddot R_x\dot Z_x-\ddot Z_x\dot R_x \\ &-\dot\gamma(\dot R_x^2+\dot Z_x^2+2R_x^2)] \\ &+\tfrac{1}{2}(a\dot c-c\dot a)(\dot R_x^2-\dot Z_x^2)\sin(2\gamma) \\ &+(a\dot c-c\dot a)\dot R_x\dot Z_x\cos(2\gamma)\}B^\phi.\end{aligned} \tag{30}$$

Taking the helical limit of Eq. (30), and using Eq. (12), recovers the constraint for the helical case, Eq. (C3). In the cylindrical limit all of the ϕ derivatives vanish, and the right-hand side reduces to $R_x^2(c^2-a^2)B^\alpha$. In particular, for a cylindrical geometry with vanishing current at the X point we recover the well-known condition that the flux surfaces must cross at right angles.

VI. DISCUSSION

The derivative of the helical flux with respect to the toroidal flux, $d\Psi_h/d\Psi_t = 1/q_h$, vanishes at a rational magnetic surface. On an unbroken rational magnetic surface, the gradient of the helical flux is zero everywhere. If the gradient of the pressure is finite at such a surface, $dp/d\Psi_h$ is singular there (it goes like q_h). It follows from Eqs. (16) and (20) that the current is singular, unless the resonant Fourier components of the Jacobian vanish there. Vanishing of the resonant Fourier components of the Jacobian on a rational surface is equivalent to $\oint dl/B$ being constant on the surface, where the integral is evaluated around a closed field line. This condition is generally not satisfied. There have been a number of discussions of this problem (see, for example, the discussion in Ref. 3). It has even been suggested that this problem implies that three-dimensional equilibria do not exist.[2]

In a more realistic treatment of three-dimensional fields, the rational surfaces break up to form islands. The infinite set of closed lines of the rational surface is replaced by a finite set of closed lines (the x lines and o lines). On the separatrix, the gradient of Ψ_h vanishes only at the x lines. A finite value of ∇p on the separatrix (away from the x line) now implies that $dp/d\Psi_h$ is finite. Since p must be constant on the flux surfaces (i.e., p must be a function of Ψ_h alone), it follows that ∇p must vanish at the x line. Our analysis shows that the pressure-driven current is well behaved in the neighborhood of the separatrix and, in fact, vanishes at the x line.

These results suggest that MHD equilibrium codes that allow island formation will be, at least in some ways, better behaved than those that assume good flux surfaces. The constraint that flux surfaces can be preserved forces the appearance of singular pressure-driven currents, unless artificial flat spots are placed in the pressure profile at the low-order rational surfaces. This effect is absent in a more realistic treatment. Even for codes that do allow island formation, however, accuracy can be expected to deteriorate in the neighborhood of a separatrix. The shape of the flux surfaces has a singularity, coming into a corner at the x line. Flux surface averages near the separatrix are dominated by the x line. The Pfirsch–Schlüter current is forced to zero near the x line. Our explicit analytical solution could be used by equilibrium codes to improve their accuracy in the neighborhood of the separatrix, much as codes now often make use of expansions around the magnetic axis to improve their treatment of equilibria there. Codes using magnetic coordinates could directly incorporate our analytical solution for these coordinates near an x line, where the coordinates are singular. Magnetic coordinates are presently used for both equilibrium[1,11] and transport[12,13] calculations.

Our solution shows that pressure-driven currents are strongly modified by the presence of a separatrix. This can be expected to be an important effect in the determination of self-consistent three-dimensional stellarator equilibria, and in the calculation of saturated finite-beta tearing modes.

ACKNOWLEDGMENT

This work was supported by the U.S. Department of Energy under Contract No. DE-AC02-76-CHO-3073.

APPENDIX A: MAGNETIC Θ COORDINATE NEAR THE x LINE

In this appendix, we give the details of the algebra for the calculation of the magnetic coordinate Θ near the x line. We first consider the toroidal component of the magnetic field. Equations (4) and (9) give

$$\mathbf{B}\cdot\nabla\phi = \frac{2q_h\rho(\partial\Theta/\partial\alpha)}{\mathscr{J}^\rho}, \qquad \text{(A1)}$$

where $q_h \equiv d\Psi_t/d\Psi_h$ is the safety factor,

$$\mathscr{J}^\rho = (\nabla\rho\times\nabla\alpha\cdot\nabla\phi)^{-1} = \frac{\partial\mathbf{x}}{\partial\rho}\times\frac{\partial\mathbf{x}}{\partial\alpha}\cdot\frac{\partial\mathbf{x}}{\partial\phi} \qquad \text{(A2)}$$

is the Jacobian of the transformation from Cartesian coordinates to the helical–hyperbolic (ρ,α,ϕ) coordinates, and $\mathbf{x} = R\mathbf{e}_R + Z\mathbf{e}_Z$ is the position vector. The transformation equations (7) and (8) allow straightforward evaluation of $\mathscr{J}^\rho$ and give

$$\mathscr{J}^\rho = -\rho Rac. \qquad \text{(A3)}$$

If we assume that the toroidal magnetic field does not vanish on the x line, and write $R\,\mathbf{B}\cdot\nabla\phi = \mathbf{B}_0(\phi)$ to lowest order, then Eqs. (A1)–(A3) determine Θ up to an integration constant as

$$\Theta = -acB_0\alpha/(2q_h) + \Theta_1(\rho,\phi). \qquad \text{(A4)}$$

The integration constant is determined in terms of B^α from the equation

$$\frac{1}{q_h}B^\phi = B^\theta = B^\alpha\frac{\partial\Theta}{\partial\alpha} + B^\phi\frac{\partial\Theta}{\partial\phi}.$$

This gives

$$\frac{\partial\Theta_1}{\partial\phi} = \frac{1}{q_h} + \frac{acR}{2q_h}B^\alpha + \frac{\alpha}{2q_h}\frac{\partial}{\partial\phi}(acB_0). \qquad \text{(A5)}$$

Now we make use of the relation

$$\frac{\partial}{\partial\phi}(acB_0) = 0,$$

which states that if a flux tube is followed in the ϕ direction, the toroidal flux through it must be conserved. (An analogous expression is valid in the neighborhood of a magnetic axis.) Another way to obtain this expression is to use the coordinate transformations (7) and (8) to show that, as long as the Cartesian components of $\mathbf{B}$ are analytic functions of position, the leading-order piece of B^α can depend on α only through $\cosh(\alpha)$ and $\sinh(\alpha)$ and cannot have a dependence that is linear in α. It follows that the term linear in α in Eq. (A5) must vanish. The same analysis also shows that to leading order B^α is independent of ρ, $B^\alpha \approx B^\alpha(\phi)$. Equation (A5) therefore gives

$$\Theta_1 = \frac{1}{q_h}\left(\phi + \frac{1}{2}\int_0^\phi acRB^\alpha\,d\phi'\right). \qquad \text{(A6)}$$

In this solution we have discarded a constant of integration which is a function only of ρ, and which does not affect the value of the magnetic field in Eq. (4).

APPENDIX B: THE PENDULUM

The magnetic field line equations for a magnetic field of the form of Eq. (4) are Hamilton's equations, where ϕ plays the role of time, Ψ_t and Θ are the canonical coordinates, and Ψ is the Hamiltonian. Magnetic coordinates correspond to action-angle variables. Our solution for magnetic coordinates near a separatrix can therefore be checked against soluble Hamiltonian systems. In particular, in the narrow island limit we should recover the action-angle variables for a pendulum. In this appendix we show that this is the case. We derive expressions for the magnetic angle Θ, and the safety factor q of a magnetic system whose flux contours in the R-Z plane are identical to the phase portrait of a mechanical pendulum.

Let

$$\psi_h = \tfrac{1}{2}G(R-R_x)^2 - H(1+\cos Z) \qquad \text{(B1)}$$

(G, H, R_x constant) define a poloidal flux function, and write the magnetic field in (R,Z,ϕ) coordinates as

$$\mathbf{B} = \nabla R\times\nabla Z + \nabla\phi\times\nabla\Psi_h. \qquad \text{(B2)}$$

The magnetic field lines satisfy

$$\frac{dR}{d\phi} = \frac{\mathbf{B}\cdot\nabla R}{\mathbf{B}\cdot\nabla\phi} = -\frac{\partial\Psi_h}{\partial Z},$$

$$\frac{dZ}{d\phi} = \frac{\mathbf{B}\cdot\nabla Z}{\mathbf{B}\cdot\nabla\phi} = \frac{\partial\Psi_h}{\partial R},$$

which are Hamilton's equations for a mechanical system with Hamiltonian $\Psi_h(R,Z)$, canonical phase-space coordinates R ("momentum") and Z ("position"), and the angle ϕ interpreted as time. The Hamiltonian is that for the pendulum. Contours of the flux function Ψ_h have a separatrix connecting two X points, at $(R=R_x, Z=\pi)$ and $(R=R_x, Z=-\pi)$. The separatrix contour is described by $\Psi_t = 0$. Flux contours with $\Psi_h < 0$ lie inside the separatrix; contours with $\Psi_h > 0$ lie outside the separatrix.

The problem of finding magnetic coordinates for the magnetic system defined in Eqs. (B1) and (B2) is equivalent to the problem of finding action-angle variables for the associated Hamiltonian. That is, a magnetic angle Θ, and a magnetic flux function Ψ_t, are sought in terms of which Eq. (B2) can be written in canonical form Eq. (4), where $\Psi(\Psi_t) = \Psi_h[R(\Psi_t,\Theta), Z(\Psi_t,\Theta)]$. The magnetic field line equations then become

$$\frac{d\Psi_t}{d\phi} = -\frac{\partial\Psi_h}{\partial\Theta},$$

and

$$\Theta = \phi/q_h + \Theta_0.$$

The derivation of action-angle variables for the pendulum Hamiltonian can be found in many of the standard textbooks of classical mechanics (see, e.g., Ref. 14). Results are conveniently expressed in terms of the parameter

$$k^2 = 1 + \Psi_h/(2H). \qquad \text{(B3)}$$

Values of $k<1$ label surfaces that lie inside the separatrix, while values of $k>1$ label surfaces that lie outside the separatrix. Then

$$\Theta(Z;k<1)=\frac{q_0}{q_<}F\left[\sin^{-1}\left(\frac{1}{k}\sin\frac{Z}{2}\right)\Big|k^2\right], \tag{B4}$$

where F is the incomplete elliptic integral of the first kind, $q_0 = 1/\sqrt{GH}$ is the safety factor at the O point $(R = R_x, Z = 0)$, and

$$q_< = F(\pi/2|k^2)2q_0/\pi \tag{B5}$$

is the safety factor for an arbitrary surface with $k<1$. Similarly,

$$\Theta(Z;k>1) = (q_0/q_>)F(Z/2|1/k^2)/k, \tag{B6}$$

where

$$q_> = F(\pi/2|1/k^2)q_0/(k\pi). \tag{B7}$$

The expressions for the Θ and q given by Eqs. (B4)–(B7) are valid everywhere in the R-Z plane. To compare the general results in the main body of our paper with the specialized model of this appendix it is necessary to expand the exact equations (B4)–(B7) about the X points $(k = 1, Z = \pm\pi)$. Since the analysis for $k<1$ and $k>1$ are very similar, we present an outline only for the notationally simpler case $k>1$.

To calculate the safety factor in the neighborhood of the X point, we use the well-known limiting behavior of the complete elliptic integrals in the limit as $k\to 1$:

$$F(\pi/2|1/k^2)\approx\log(4/\sqrt{k^2-1}), \quad k\to 1^+. \tag{B8}$$

Substituting into (B4) and (B6), using Eq. (B3) to write k^2 in terms of Ψ_h, and identifying Eq. (B1) with Eq. (5) to give $G = 2/a^2$, $H = 2/c^2$, easily verifies Eq. (15) of the main text. [In Eq. (15) we must set $n_x = 2$ for $k<1$ and $n_x = 1$ for $k>1$.]

The limiting behavior of the magnetic angle is slightly more tricky. For this, in addition to using Eq. (B8), we must use an expansion of the incomplete elliptic integrals about $Z = \pi$ and $k = 1$. To this end, we use the result[15]

$$F(Z/2|1/k^2) = F(\pi/2|1/k^2) - F(\zeta|1/k^2), \tag{B9}$$

where

$$\cos(\alpha)\tan(Z/2)\tan(\zeta) = 1 \tag{B10}$$

and $\sin^2(\alpha) = 1/k^2$. Since $k\approx 1$, $F(\zeta|k^2)$ can be replaced, approximately, by $\log\sqrt{(1+\sin\zeta)/(1-\sin\zeta)}$, where $\sin(\zeta)$ is obtained from rearranging Eq. (B10) in the form

$$\sin^2(\zeta) = \frac{k^2\sin^2(\delta Z/2)}{[(k^2-1)+\sin^2(\delta Z/2)]}.$$

On the right-hand side, we use the small argument approximation to the sine function, write k^2 in terms of Ψ_h using Eq. (B3), and expand Ψ_h about the X point as $\Psi_h \approx (\delta R)^2/a^2 - (\delta Z)^2/c^2$. Pulling these pieces together obtains

$$F(\zeta|k^2)\approx\log\sqrt{[c(\delta R)+a(\delta Z)]/[c(\delta R)-a(\delta Z)]}. \tag{B11}$$

The leading-order behavior of the magnetic angle in the vicinity of the X point obtained in the main text is verified by direct substitution of Eqs. (B8), (B9), and (B11) into Eq. (B4).

APPENDIX C: HELICAL AND CYLINDRICAL SYMMETRY

In this appendix we use the Grad–Shafranov equation to give an alternative derivation of the constraint due to Ampère's law for helical and cylindrical systems. We adopt the notation of Ref. 16 for the magnetic field in helical geometry. In terms of cylindrical coordinates (r,θ,z) we define the variable $u\equiv l\theta - hz$ and the vector

$$\mathbf{u} = (l\hat{\mathbf{z}} + hr\hat{\theta})/(l^2 + h^2r^2),$$

where l and h are given constants. All quantities are taken to be functions of r and u. The magnetic field can be expressed in terms of two arbitrary functions, $f(r,u)$ and $F(r,u)$,

$$\mathbf{B} = f(r,u)\mathbf{u} + \mathbf{u}\times\nabla F(r,u).$$

It follows that Ampère's law may be written

$$\mathbf{J} = \left(\frac{l^2+h^2r^2}{r^2}\mathscr{L}F + \frac{2hl}{l^2+h^2r^2}f\right)\mathbf{u} + \mathbf{u}\times\nabla(-f), \tag{C1}$$

where

$$\mathscr{L} = r\frac{\partial}{\partial r}\frac{r}{l^2+h^2r^2}\frac{\partial}{\partial r} + \frac{\partial^2}{\partial u^2}. \tag{C2}$$

In this formalism, F is a helical flux function (it is proportional to our Ψ_h, but not equal to it). To apply the formalism to a separatrix, we take F to be of the same form as the ψ_h of Eqs. (6) and (7), with $a\to A$ and $c\to C$. In this geometry, R and Z are Cartesian coordinates,

$$\phi = z,$$
$$R - r_x = r\cos(\theta) - r_x\cos(\theta_x),$$
$$Z - Z_x = r\sin(\theta) - r_x\sin(\theta_x),$$

where r_x is the (z independent) radius of the x line, and $\theta_x = hz/l$ is the angular location of the x line as a function of z. (In dropping an additive constant from the expression for θ_x we have chosen our coordinate origin in the z direction.) It follows that

$$\xi = r\cos(\theta+\gamma) - r_x\cos(\theta_x+\gamma),$$
$$\eta = r\sin(\theta+\gamma) - r_x\sin(\theta_x+\gamma).$$

For a helically symmetric field γ takes the form $\gamma = -hz/l + \gamma_0$, where γ_0 is a constant.

Substituting our expression for F into Eqs. (C1) and (C2), we find

$$\begin{aligned}\frac{\mathbf{J}\cdot\mathbf{u}}{\mathbf{u}\cdot\mathbf{u}} = &-\left(\frac{1}{A^2}+\frac{1}{C^2}\right)\frac{h^2r_x^2}{l^2}\cos(2\gamma_0)\\ &+\left(\frac{1}{A^2}-\frac{1}{C^2}\right)\frac{h^2r_x^2+2l^2}{l^2}\\ &+\frac{2hl}{l^2+h^2r_x^2}f,\end{aligned} \tag{C3}$$

where the A and C in this expression differ from the a and c in the rest of the paper only by an overall normalization. Equation (C3) is the desired constraint. If we set $l = 1$ and $h = 0$, we obtain the equation for cylindrical symmetry. In particular, for a vacuum field ($J = 0$) we obtain the well-known constraint that $A = C$ for a separatrix with cylindrical symmetry.

APPENDIX D: METRIC ELEMENTS

We calculate the elements of the covariant metric tensor by substituting Eqs. (7) and (8) into Eq. (27). The results are as follows:

$$g_{\rho\rho} = \cosh(2\alpha)(c^2 + a^2)/2 + (a^2 - c^2)/2,$$

$$g_{\rho\alpha} = \sinh(2\alpha)(c^2 + a^2)\rho/2,$$

$$\begin{aligned} g_{\rho\phi} = {} & [\sinh(\alpha)\sin(\gamma)c + \cosh(\alpha)\cos(\gamma)a]\dot{R}_x \\ & - [\cosh(\alpha)\sin(\gamma)a - \sinh(\alpha)\cos(\gamma)c]\dot{Z}_x \\ & + [\cosh(2\alpha)(c\dot{c} + a\dot{a}) + a\dot{a} - c\dot{c}]\rho/2, \end{aligned}$$

$$g_{\alpha\alpha} = [\cosh(2\alpha)(c^2 + a^2) + c^2 - a^2]\rho^2/2,$$

$$\begin{aligned} g_{\alpha\phi} = {} & \rho\{[\cosh(\alpha)\sin(\gamma)c + \sinh(\alpha)\cos(\gamma)a]\dot{R}_x \\ & - [\sinh(\alpha)\sin(\gamma)a - \cosh(\alpha)\cos(\gamma)c]\dot{Z}_x\} \\ & + \rho^2[\sinh(2\alpha)(c\dot{c} + a\dot{a})/2 - \dot{\gamma}ac], \end{aligned}$$

$$\begin{aligned} g_{\phi\phi} = {} & \dot{R}_x^2 + \dot{Z}_x^2 + R_x^2 \\ & + 2\rho\{[-\cosh(\alpha)\sin(\gamma)\dot{\gamma}a \\ & + \sinh(\alpha)\cos(\gamma)\dot{\gamma}c \\ & + \dot{c}\sinh(\alpha)\sin(\gamma) + \dot{a}\cosh(\alpha)\cos(\gamma)]\dot{R}_x \\ & - [\sinh(\alpha)\sin(\gamma)\dot{\gamma}c + \cosh(\alpha)\cos(\gamma)\dot{\gamma}a \\ & + \dot{a}\cosh(\alpha)\sin(\gamma) - \dot{c}\sinh(\alpha)\cos(\gamma)]\dot{Z}_x\}. \end{aligned}$$

[1]A. Reiman and H. Greenside, Comput. Phys. Comm. **43**, 157 (1986).
[2]H. Grad, Phys. Fluids **10**, 137 (1967).
[3]L. S. Solov'ev and V. D. Shafranov, in *Reviews of Plasma Physics*, edited by M. A. Leontovich (Consultants Bureau, New York, 1970), Vol. V, p. 1.
[4]A. H. Boozer, Phys. Fluids **24**, 1999 (1981).
[5]S. P. Auerbach and A. H. Boozer, Phys. Fluids **23**, 2396 (1980).
[6]A. H. Reiman and A. H. Boozer, Phys. Fluids **27**, 2446 (1984).
[7]J. R. Cary and M. Kotschenreuther, Phys. Fluids **28**, 1392 (1985).
[8]J. M. Greene and J. L. Johnson, Phys. Fluids **5**, 510 (1962).
[9]S. Hamada, Nucl. Fusion **1**, 23 (1962).
[10]R. H. Rand, *Computer Algebra in Applied Mathematics: An Introduction to MACSYMA*, Research Notes in Mathematics (Pitman, London, 1984), Vol. 94.
[11]T. C. Hender, B. A. Carreras, L. Garcia, J. A. Rome, and V. E. Lynch, J. Comput. Phys. **60**, 76 (1985).
[12]A. H. Boozer and G. Kuo-Petravic, Phys. Fluids **24**, 851 (1981).
[13]G. Kuo-Petravic, A. H. Boozer, J. A. Rome, and R. H. Fowler, J. Comput. Phys. **51**, 261 (1983).
[14]A. J. Lichtenberg and M. A. Lieberman, *Regular and Stochastic Motion* (Springer, Berlin, 1983), Sec. 1.3.
[15]W. Gautschi, in *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. Stegun (National Bureau of Standards, Washington, DC, 1964), p. 295.
[16]C. Mercier, *The Magnetohydrodynamic Approach to the Problem of Plasma Confinement in Closed Magnetic Configurations*, Lectures in Plasma Physics (Commission of the European Communities, Luxembourg, 1974), p. 10.