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TOKAMAK ERROR FIELDS AND LOCKED MODES

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Tokamak Error Fields and Locked Modes

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Abstract

The effects of externally applied, resonant magnetic field perturbations on tokamak plasmas are discussed. An analytical model assuming tokamak ordering and narrow islands clarifies the conditions under which error fields are amplified or diminished by self-consistent effects. A strong amplification of error fields near marginal tearing stability is found to broaden the range of parameters over which deleterious tearing effects are seen. Three-dimensional numerical solutions indicate that saturated tearing mode island widths can be sensitive to the presence of small nonaxisymmetric perturbations. It is argued that the theoretical conclusions are consistent with observations in error compensation experiments, and are also consistent with observations of enhanced growth for locked modes.

In this paper we discuss the effects of small, nonaxisymmetric magnetic field perturbations on tokamak plasmas. We focus on perturbations which can resonate with low order rational surfaces in the plasma and produce magnetic islands ($m = nq$ for the poloidal and toroidal mode numbers m, n .) Error fields of this sort are produced in present day tokamaks by such things as finite tolerances in installation of the poloidal field coils, the presence of bus bars, etc. Typical magnitudes of such fields are $\delta B/B_t \approx 10^{-4}$, where B_t is the toroidal field. Over the past few years, experimental evidence has accumulated that error fields of this magnitude can produce significant effects on tokamak discharges.

A coil which is capable of partially compensating the known error field has been placed on DIII-D. This error compensation coil is believed to improve the general performance of the device. In particular, a systematic dependence of the low density locked mode threshold on the error compensation field has been documented.¹

On Asdex, heat deposition on the divertor plates is nonaxisymmetric for rf heated discharges, even in the absence of locked modes. The nonaxisymmetric deposition is believed to be due to the presence of islands produced by error fields.²

On JFT-2M, small fields produced by the ergodic limiter coil are found to systematically affect the threshold power for the L-H transition.³

In a number of tokamaks, rotating tearing modes are found to lock onto error fields.^{4,5} Locking exacerbates nonaxisymmetric heat deposition. It is also generally believed that locked modes disrupt more readily than rotating tearing modes.

These observations raise some serious concerns for the next generation of tokamaks. Heat load on the divertor plates is already an issue for these devices. Nonaxisymmetric heat deposition makes the situation worse by increasing the peak heat load. Also, the divertor plates can only tolerate a limited number of disruptions due to ablation of material from the divertor plates during disruptions. Disruptivity is therefore an issue.

In addition to the practical issues, error field effects also provide a testing ground for some interesting physics issues. A small, resonant magnetic field perturbation affects the plasma significantly only in a narrow region about the rational surface, allowing us to test our understanding of the physics of magnetic islands. We will also see that the presence of an infinitesimal non-

axisymmetric perturbation provides a link between three-dimensional equilibrium theory and stability theory, suggesting an equilibrium approach to the computation of saturated tearing modes.

This paper will discuss several models for error field effects in tokamaks. We will start with some simple models to see what physics we can extract from them and what their limitations are. We will work our way up in complexity, and at the end will describe some three-dimensional numerical computations.

One widely used model for error field effects represents the plasma current by a single circular current filament. The vacuum field produced by this current filament is superposed on the vacuum error field to produce a model field, whose field lines are followed to determine flux surfaces and islands. For the known error fields in present day experiments, this typically predicts island widths which are a few percent of the minor radius. Although the calculated widths are probably not large enough to have a significant effect on a tokamak discharge, the widths predicted by this very crude model are sufficiently large to suggest that it is worth doing a more sophisticated calculation to determine the island widths more accurately.

The circular filament model neglects the self-consistent response of the plasma currents to the presence of the error field. This response can be crudely incorporated in the model. At zero β , currents follow the perturbed magnetic field lines. This can be modeled by distorting the circular filament to follow the magnetic axis. When this calculation was applied to nonaxisymmetric experiments on the ST tokamak,⁶ and on PLT,⁷ it was found that the computed island widths were greatly reduced from those calculated with a circular filament. The results suggest that any model with purely axisymmetric plasma currents is unreliable, that self-consistent currents can be important. The results have also been widely interpreted as showing that tokamaks are self-healing in the presence of error fields, that they always shield out nonaxisymmetric perturbations. (Although references 6 and 7 make no such claim.) We will see that this is not the case, that self-consistent plasma effects can amplify error fields.

There is at least one case where it is clear that an external perturbation will be amplified. If the profile is near marginal stability for tearing, the perturbation will feed off the free energy for the tearing mode. To see that this is so, we consider a sketch of a marginal tearing eigenmode in a cylinder (the

lower curve in Fig. 1). The radial component of the field goes to zero at the boundary and at the magnetic axis, and it is finite in between. At marginal stability (zero growth rate), the tearing eigenmode is an equilibrium solution. A knowledge of the tearing eigenmode therefore allows us to determine what equilibria look like in the neighborhood of marginal stability. The upper curve in Fig. 1 is a sketch of an equilibrium solution, with an error field, just below marginal stability. It, too, must go to zero at the magnetic axis. At the edge, it has a finite value determined by the external perturbation. In between, its shape must be close to that of the nearby marginal eigenmode. It is clear from this sketch that we get large amplification at the rational surface. (In contrast, the vacuum error field $B_r \propto r^{m-1}$, where m is the poloidal mode number.) In the absence of the error field, there would be no magnetic island below the tearing threshold. The presence of an error field effectively broadens the range of parameters over which we see deleterious tearing effects.

The filament model suggested that tokamak plasmas are sometimes self-healing. We have argued that plasmas should amplify an external perturbation in some neighborhood of marginal tearing instability. We will now turn to a somewhat more sophisticated analytical model. One focus will be to gain a better understanding of the conditions under which we expect a tokamak plasma to be self-healing.

Our analytical calculation assumes narrow islands and tokamak ordering. The solution for the perturbed helical flux function outside the islands is determined by the tearing mode equation for the exterior region:

$$\frac{d}{dr} r \frac{d\psi}{dr} - \frac{m^2}{r^2} \psi = \frac{j_0 R}{B_z(z - n/m)} \psi, \quad (1)$$

with the boundary condition

$$\psi \rightarrow \epsilon$$

at the edge. (ϵ is the given external perturbation.) This is the perturbed equilibrium equation. The perturbed current in the island, determined by Faraday's law, gives a jump condition across the island of the form

$$r_o \psi'(r_o) - r_i \psi'(r_i) = I(w),$$

where r_o, r_i are the island edges and $I(w)$ is related to the perturbed island current. The resulting model is a generalization of the usual nonlinear tearing

mode theory⁸⁻¹⁰ to include the effects of a fixed external perturbation. Details of the calculation are presented in Ref. 11.

To make contact with the conventional Δ' calculation, we let ψ_1, ψ_2, ψ_i satisfy Eq. (1) with

$$\begin{aligned}\psi_1(r=a) &= 0, & \psi_1'(r=a) &= 1, \\ \psi_2(r=a) &= 1, & \psi_2'(r=a) &= 0,\end{aligned}$$

$$\psi_i \longrightarrow r^m \text{ as } r \longrightarrow 0.$$

We write

$$\psi = \begin{cases} a_1 \psi_1 + \epsilon \psi_2 & \text{for } r > r_o, \\ a_i \psi_i & \text{for } r < r_i. \end{cases}$$

Applying the jump condition across the island, we obtain an eigenvalue equation for w of the form:

$$\alpha w^3 - \Delta' w^2 = \pm \sigma' \epsilon, \quad (2)$$

where

$$\sigma' \equiv \frac{4}{\psi_0''} [\psi_1'(r_o)/\psi_1(r_o) - \psi_2'(r_o)/\psi_2(r_o)] \psi_2(r_o).$$

and where the $\pm$ sign corresponds to the phase of the solution. In this expression, ϵ measures the strength of the perturbation at the boundary (the error field). The coefficient Δ' is the usual parameter measuring the free-energy available to drive tearing

$$\Delta' = \psi_1'(r_s)/\psi_1(r_s) - \psi_i'(r_s)/\psi_i(r_s),$$

where r_s corresponds to the rational surface. The tearing mode is unstable for $\Delta' > 0$, and stable for $\Delta' < 0$. The αw^3 term is primarily determined by the nonlinear modification of Δ' in the presence of an island.

Figures 2 and 3 show schematically what the roots of the eigenvalue equation look like without and with an error field. The quantity $\psi(r_s)$ is plotted as a function of a profile parameter, with Δ' assumed to increase monotonically as a function of the parameter. We plot ψ at the rational surface rather than w to retain the phase information.

Figure 2 shows the solution in the absence of an error field. For $\Delta' < 0$ there is a unique solution, corresponding to a stable, cylindrically symmetric equilibrium. For $\Delta' > 0$, the cylindrically symmetric equilibrium is unstable.

There are also solutions corresponding to saturated tearing modes. These are stable, nonsymmetric equilibria with islands. As $\Delta' \rightarrow 0$ from the right, the island width goes to zero. The point $\Delta' = 0$ corresponds to a bifurcation point of the solution.

When $\epsilon > 0$, the solution of Eq. (2) is as shown in Fig. 3. There is still a unique, stable solution for $\Delta' < 0$, but the equilibrium is now a nonsymmetric one with an island. For large Δ' there are again three solutions. The external perturbation breaks the bifurcation at $\Delta' = 0$, so that the solution now consists of two independent branches. The solution for $\Delta' < 0$ now goes smoothly into the locked mode solution for $\Delta' > 0$. This is the branch that we are interested in.

One thing that the picture of Figure 3 suggests is that a natural way to numerically compute the locked mode solution in three dimensions is to use a three-dimensional equilibrium code to track the solution in the presence of a nonaxisymmetric perturbation as we go from the stable regime to the unstable one. That is our approach to the calculation of locked modes. The picture of Figure 3 also has implications for the calculation of saturated tearing modes, even in the absence of an error field. The conventional approach to the calculation of saturated tearing modes, indicated in Fig. 4a, is to perturb an unstable axisymmetric equilibrium and use a time-dependent code to follow the tearing mode as it grows and saturates. If the saturated tearing mode is desired for several different values of the plasma parameters, the calculation is repeated for a corresponding number of different equilibria. The alternative approach indicated in Fig. 4b is to apply a small nonaxisymmetric perturbation and follow the equilibrium solution from the tearing stable regime into the unstable regime. This gives a direct calculation of the saturated tearing mode for a range of parameters. If desired, the finite ϵ solution for a given value of the profile parameter can be tracked to $\epsilon = 0$, as indicated in the figure.

One thing that we would like to understand about the solution of Fig. 3 is whether the plasma amplifies or diminishes the error field when $\Delta' < 0$. To get a feeling for that, we consider a special case where things simplify somewhat. We assume that the island is in the vacuum region outside the plasma. We get

$$\sigma' = \frac{8m}{\psi_0'' r_s} \frac{1}{(r_s/a)^m - (r_s/a)^{-m}}, \quad \alpha = 0,$$

where we impose the error field at $r = a$. This gives an explicit expression for the island width,

$$w^2 = -16 \frac{\epsilon}{\psi_0''} \left(\frac{r_s}{a} \right)^m \frac{\Delta'_v}{\Delta'}, \quad (3)$$

where

$$\Delta'_v = \frac{2m}{r_s} \frac{1}{(r_s/a)^{2m} - 1}$$

is Δ' for $j'_0 \rightarrow 0$ in Eq. (1). For $\Delta' = \Delta'_v$, we get the usual error field in vacuum. We can get amplification or self-healing, depending on whether $|\Delta'|$ is greater than or less than $|\Delta'_v|$.

The result is intuitively plausible. When Δ' is sufficiently large and negative, the plasma is self-healing. When $\Delta' < 0$ approaches zero, we get amplification. There is a critical value of Δ' at which the island width is just that due to the vacuum error field. As a particular example, for an $m = 2$ island with $r_s/a = .3$, $\Delta'_v \approx -13$.

Our formula for w , Eq. (3), gives $w \rightarrow \infty$ as $\Delta' \rightarrow 0$. This is because we have assumed that the island lies outside the plasma. There is no redistribution of current in the island as it increases in width. As $\Delta' \rightarrow 0$, we approach marginal stability for the external kink. For an island in the plasma interior, the width remains finite as $\Delta' \rightarrow 0$ due to the αw^3 term in Eq. (3). The island width gets large in this limit, $w \propto \epsilon^{1/3}$ rather than $\epsilon^{1/2}$.

We turn now to numerical calculations. The focus here will be the unstable regime. We present here only a few illustrative calculations. A forthcoming paper will present an extensive set of numerical computations.¹²

As discussed above, we use a three-dimensional equilibrium code for our numerical calculations. We solve the three-dimensional equilibrium equation,

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

using the PIES code,^{13,14} which is capable of handling islands and stochastic regions.

As for any equilibrium solution, we need to specify two free functions to determine the pressure and current profiles. We specify a pressure profile, $p(\rho)$, and a quantity we will call μ ,

$$\mu(\rho) \equiv (\mathbf{j} \cdot \mathbf{B} / B^2),$$

where ρ is a coordinate that is constant on flux surfaces, and $\langle \rangle$ denotes an average over a flux surface. The code allows stochastic regions and islands in the solution, and it flattens the profiles in those regions. The profiles on the good flux surfaces must also be adjusted to insure that there are no discontinuities at the edges of the flattened regions. To handle the profile adjustments, we define ρ itself to be constant in the islands and stochastic regions. We define ρ on the midplane by $d\rho/dR = 1$ on the good surfaces, and $d\rho/dR = 0$ in the islands and stochastic regions, where R is the major radius. We extend ρ off the midplane by taking it to be constant on the flux surfaces. As the code iterates, the widths of the islands and stochastic regions adjust self-consistently. At each iteration, a diagnostic in the code automatically determines where those regions are. The coordinate ρ is then recalculated, and the profiles are correspondingly adjusted.

The calculations we show all have zero β ($p = 0$). We use the current profiles of Furth et al.,¹⁵

$$j(\rho) = j_0 \left[1 + (r/r_0)^{2\gamma} \right]^{-(1+1/\gamma)}. \quad (4)$$

These current profiles have been used extensively for tearing mode studies. We take $r_0/a = .6$, and we choose j_0 so that q on axis is 1.05.

In addition to specifying the profiles, we also need to give a boundary condition. We specify the normal component of $\mathbf{B}$ on a bounding reference surface. This field can be calculated from a specified set of three-dimensional coils outside the bounding surface.

Although we can solve the fully three-dimensional problem in a torus, it is useful to also look at some solutions in a cylinder. Such solutions are helpful in understanding the physics, because the island width is tied directly to the radial component of the field ($w \propto |B_r|^{1/2}$). We will look first at helical solutions in a long, thin cylinder ($R/a = 20$) for an $m = 2$, $n = 1$ mode, taking $\gamma = 4$ in Eq. (4). The mode is unstable for our choice of parameters. Figure 5 shows the equilibrium value of $R_0 B_r / a B_0$ as a function of r/a for several different values of B_r at the edge. The curve with $B_r = 0$ at $r = a$ corresponds to the saturated tearing mode in the absence of an error field. The corresponding normalized value of B_r at the rational surface is 1.6×10^{-4} , which gives an island width of about 5%. In addition to $B_r = 0$ at the edge, we also show cases with normalized B_r values of 10^{-4} and 3×10^{-4} at the edge. In the absence of a self-consistent plasma response, B_r would decay

linearly away from the boundary. For $R_0 B_r(r=a)/a B_\phi = 10^{-4}$, for example, the vacuum error field would have a magnitude at the rational surface about half that of the saturated mode. Instead, we find that the self-consistent plasma response strongly amplifies the error field, so that the field at the rational surface is about 5 times that at the edge, and about 3 times what it is in the absence of an error field. Multiplying the field at the edge by a factor of 3 gives little change in the shape of the eigenfunction, so that the field at the rational surface is now about 4 times what it is at the boundary, and about 8 times what it is in the absence of an error field.

Now we turn to some toroidal, fully three-dimensional solutions. Figures 6 and 7 show Poincare plots for solutions with $R/a = 3$ and $\gamma = 1$, without and with an error field. (We caution that the origin of our coordinate system does not lie on the magnetic axis, so the region about the axis looks like an island, but is not an island.) The tearing mode is unstable for these parameters. In the absence of an error field there are saturated islands at the $q = 2$ and $q = 3$ rational surfaces, with the total island width across the midplane about 6%.

The solution in Fig. 7 has an error field imposed with resonant $n = 1$ and $n = 2$ Fourier components. The magnitude of the Fourier components were calculated from a small shift and elliptical deformation of a nearly circular poloidal field coil at $R = 6a$. The coil current and shift were chosen to approximately reproduce the reported $n = 1$ error field spectrum on DIII-D, with an $n = 1, m = 2$ amplitude of about $5.5 \times 10^{-5} B_t$.¹ (The shift is 0.5%, and the current is approximately that required by the Shafranov formula for radial force balance.¹⁶) The elliptical deformation was also taken to be .5%. This is comparable to the maximum measured elliptical deformation of the TFTR poloidal field coils. With the imposed error field, the islands are now larger and more numerous. The total island width across the midplane is now about 23%.

Finally, we discuss the correspondence between our theoretical results and some of the experimental observations.

The DIII-D tokamak encounters a locked mode at low density. The density threshold for this mode has been found to depend systematically on the field in the error compensation coil. In particular, using the error compensation coil to reduce the ambient error field makes it possible to reach lower densities. This behavior is consistent with our conclusion that the presence of

an error field broadens the range of plasma parameters over which deleterious tearing effects are seen.

On a number of tokamaks, locked modes are believed to grow to larger amplitude and to disrupt more readily than rotating modes. This is also something that our calculations would lead us to expect. When a magnetic island is rotating rapidly past an error field, the growth of the island is not strongly affected by the presence of the error field. Induced wall currents can slow the mode rotation, and allow the mode to lock onto the external error field.¹⁷ The error field can then strongly affect the saturation amplitude, and therefore the subsequent evolution, of the stationary island. The absence of wall stabilization also enhances the growth of locked modes.¹⁸ The relative importance of these two effects has yet to be sorted out. Measurements of the toroidal plasma rotation on JET¹⁹ and Asdex⁵ indicate that it is globally damped to a small value in the presence of locked modes, so that flow effects can be safely neglected in calculating the subsequent evolution of the mode.

We conclude that experiment and theory are presenting us with a consistent picture indicating that error fields of the magnitude that exist in present day tokamaks are having significant effects. The theory predicts that error fields can be strongly amplified below the tearing threshold. It follows that the presence of error fields broadens the range of plasma parameters over which deleterious tearing effects are seen. The theory also predicts that the saturation amplitude of tearing modes can be sensitive to the presence of relatively small error fields. These theoretical results suggest that error field amplitudes in the next generation of tokamak experiments will affect heat deposition peaking factors on the divertor plates (through nonaxisymmetric heat deposition), and will affect disruptivity. Improved understanding of error field effects will play a role in the design of the next generation of tokamaks in terms of suggesting construction tolerances, and possibly in terms of suggesting the desirability of trim coils for tuning out residual field errors.

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References

- ¹T. Scoville et al., Bull. APS **34**, 2118 (1989).
- ²T. E. Evans, J. Neuhauser, F. Leuterer, E. R. Mueller, and the Asdex Team, Characteristics of toroidal energy deposition asymmetries in Asdex, Technical Report GA-A20076, General Atomics, 1990.
- ³A. W. Leonard et al., Bull. APS **35** (1990).
- ⁴J. A. Snipes et al., Nucl. Fusion **28**, 1085 (1988).
- ⁵H. Zohm, A. Kallenbach, H. Bruhns, G. Fussmann, and O. Klueber, Europhys. Lett. **11**, 745 (1990).
- ⁶W. Stodiek, K. Bol, H. Eubank, S. V. Goeler, and D. J. Grove, Effect of non-axisymmetric confining fields on tokamak discharges, in **Plasma Physics and Controlled Nuclear Fusion Research, Proceedings of the Fourth International Conference, Madison, Vol. I**, pages 465-478, 1971.
- ⁷R. Goldston et al., Confinement studies during neutral beam injection in PLT, in *Heating in Toroidal Plasmas*, pages 711-721, Commission of the European Communities, 1980, Proceedings of the 2nd Joint Grenoble-Varenna International Symposium - Villa Olmo - Como - Italy.
- ⁸R. B. White, D. A. Monticello, M. N. Rosenbluth, and B. V. Waddell, Phys. Fluids **20**, 300 (1977).
- ⁹R. B. White, Rev. Mod. Phys. **58**, 183 (1986).
- ¹⁰L. Zakharov, Quasilinear equilibria related to tearing modes in tokamaks, Technical Report FRCR 319, Fusion Research Center, University of Texas, Austin, Texas, 1988.
- ¹¹A. Reiman, Tokamak magnetic islands in the presence of nonaxisymmetric perturbations, to be published.
- ¹²A. Reiman and D. Monticello, Sensitivity of tokamak equilibria to the presence of nonaxisymmetric error fields — numerical computations, to be published, 1990.

- ¹³A. H. Reiman and H. S. Greenside, *Comput. Phys. Commun.* **43**, 157 (1986).
- ¹⁴A. H. Reiman and H. S. Greenside, *jcp* **87**, 349 (1990).
- ¹⁵H. P. Furth, P. H. Rutherford, and H. Selberg, *Phys. Fluids* **16**, 1054 (1973).
- ¹⁶V. D. Shafranov, *Reviews of Plasma Physics*, volume 2, pages 103–151, Consultants Bureau, New York, 1966.
- ¹⁷M. F. F. Nave and J. A. Wesson, Mode locking in tokamaks, in *Controlled Fusion and Plasma Physics (Proc. 14th Eur. Conf. Madrid, 1987)*, Vol. 11D, Pt. III, page 1103, European Physical Society, 1987.
- ¹⁸M. Persson and A. Bondeson, *Nucl. Fus.* **29**, 989 (1989).
- ¹⁹J. A. Snipes, D. J. Campbell, T. C. Hender, M. V. Hellermann, and H. Weisen, *Nucl. Fusion* **30**, 205 (1990).

Figures

FIG. 1. Sketch of a marginally stable tearing eigenmode (lower curve) and an equilibrium solution just below the tearing threshold (upper curve).

FIG. 2. Schematic plot of $\psi(r_s)$ as a function of a profile parameter for $\epsilon = 0$. We assume that Δ' increases monotonically with the profile parameter.

FIG. 3. Solution for $\psi(r_s)$ with finite ϵ . The dashed line indicates the solution in the $\epsilon = 0$ limit.

FIG. 4. Schematic view of saturated island calculation by a) conventional time-dependent methods, and b) tracking the equilibrium solution.

FIG. 5. Normalized radial field for a helical equilibrium solution with several different values of the error field.

FIG. 6. Poincare plot for a toroidal solution with $R/a = 3$, $\gamma = 1$ and no error field.

FIG. 7. Poincare plot for a toroidal solution with $R/a = 3$, $\gamma = 1$ and error field as described in the text.

Fig. 1

Fig. 2

Fig. 3

**a) conventional time-dependent
calculation**

b) equilibrium calculation

Fig. 4

Fig. 5

90T1008

Fig. 6

90T1009

Fig. 7