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Three-dimensional linear peeling-ballooning theory in magnetic fusion devices

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Ideal magnetohydrodynamics theory is extended to fully 3D magnetic configurations to investigate the linear stability of intermediate to high n peeling-ballooning modes, with n the toroidal mode number. These are thought to be important for the behavior of edge localized modes and for the limit of the size of the pedestal that governs the high confinement H-mode. The end point of the derivation is a set of coupled second order ordinary differential equations with appropriate boundary conditions that minimize the perturbed energy and that can be solved to find the growth rate of the perturbations. This theory allows of the evaluation of 3D effects on edge plasma stability in tokamaks such as those associated with the toroidal ripple due to the finite number of toroidal field coils, the application of external 3D fields for elm control, local modification of the magnetic field in the vicinity of ferromagnetic components such as the test blanket modules in ITER, etc. © 2014 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4871859>]

I. INTRODUCTION

The magnetohydrodynamic (MHD) model is inherently limited in scope and applicability by the strong assumptions behind it. Yet, despite its relative simplicity, it has been shown to be surprisingly applicable, mainly due to the strong anisotropy between the parallel and perpendicular dynamics. Furthermore, MHD theory can generally be used as a baseline for the behavior of plasma dynamics.¹ Important here are the MHD instabilities that may ultimately limit the performance of fusion devices.

There is a variety of MHD instabilities that can occur in plasma and they can be categorized in various ways: One of them is the distinction between internal instabilities, that do not disturb the plasma boundary, and external ones, that do. Alternatively, they can be global, spanning an extended range within the plasma, or localized. Lastly, another way of classification instabilities is by considering the main mechanism that drives them. These turn out to be the parallel current and the pressure gradient, hence the denotation “current driven” or “pressure driven.”^{2,3}

Two important modes of instabilities that have been identified in current devices are the *peeling mode*, which is a global, current driven mode that can be thought of as a limiting case of the external interchange mode,⁴ and the *ballooning mode*, which is a localized pressure driven mode. Note, however, that here and henceforth the words local and global indicate a localization around particular field lines versus delocalization in the entire flux surface, respectively, and are not directly connected to the radial extent. Coupled, the peeling-ballooning modes are thought to be important for the limiting behavior of some modern devices, as they are able to cause periodically erupting *edge localized modes* (ELMS). These limit the size of the pressure gradient in the *pedestal*,

which is one of the main characteristics of the high confinement *H-mode*.⁵ Therefore, it is of importance to correctly understand the physics behind the peeling-ballooning mode and to be able to simulate it accurately.

There exist fairly complete analytical theories for both the localized, pressure driven ballooning mode^{6,7} and the global, current driven peeling mode.⁸ Since the main interest for ELMS lies in describing the instabilities of the outer layers of the plasma, these theories take into account the approximate effect of the perturbation of the plasma edge. However, bringing these two theories together required some effort, since the theory of peeling modes is formulated for global modes, whereas the theory of ballooning modes employs an asymptotic, so-called “high n ” (where n refers to the toroidal mode number) ordering that is valid only for localized modes, and breaks down for more extended modes. It is clear, then, that a purely analytical theory is difficult to conceive and one has to resort to simulations.

One strategy has been to drop the high n ordering which, though useful for analytical understanding of the ballooning modes, cannot easily describe the peeling modes, and to simulate the plasma with the full MHD model without approximation in the toroidal mode number. Codes such as MISHKA⁹ and KINX¹⁰ are very successful at describing the phenomena of peeling-ballooning modes and accurate results have been obtained.¹¹ However, since these codes are not very fast, they are not always suitable for parameter studies, so a main step in this domain has been the development of the linear numerical code ELITE, that indeed employs a high- n ordering at the plasma edge, but also keeps higher order terms to correctly describe the intermediate n peeling-ballooning modes.¹²

ELITE has been successful at describing peeling-ballooning phenomena and has allowed the subsequent study of the linear properties of ELMS.^{5,13,14} However, the main limitation of ELITE and the theory behind it is the fact that it is valid only for *axisymmetric* configurations. This allows for many simplifications, yet it can present an important

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limitation to the generality of the predicted results. For example, stellarators are inherently 3D and thus need 3D theory to be accurately described. But also tokamaks, which can be approximated quite well by the assumption of axisymmetry, experience some degree of three dimensionality. The ripple due to the discrete toroidal coils, for example, breaks axisymmetry. Also, in recent years, the effects of resonant 3D fields on the edge of tokamak plasmas have received increased attention because of their capability to control the energy losses and power fluxes to plasma facing components caused by ELMS, which can lead to unacceptable erosion rates of these components in tokamak fusion reactors such as ITER.¹⁵

In this work, a full 3D theory is developed in the same spirit as the axisymmetric theory behind ELITE, yet without employing the limiting axisymmetric assumption. It differs from pure analytical 3D ballooning mode theory and 3D peeling mode theory in two ways. First, no assumptions are made on the form of the plasma perturbation, such as the *ballooning description* used to derive the general 3D ballooning mode equation.¹⁶ Second, the treatment of the plasma edge is not done in an approximate fashion, as in Ref. 7 for 2D ballooning modes,¹⁷ for 3D ballooning modes or⁸ for peeling modes: The inclusion of the effects due to the perturbation of the plasma surface is done as in ELITE, through the actual calculation of the perturbed energy of the plasma boundary and the surrounding vacuum, employing the extended energy principle.¹⁸

The structure of this paper is as follows: In the next section, the major analytical derivation of the 3D peeling-

ballooning theory is developed. This is done in steps, described in various subsections. The results, which consist of a coupled set of second-order linear differential equations whose solution provides the growth rate of the system, are then discussed in Sec. III and interesting features are pointed out, as well as the parallels with the 2D work performed earlier. After that, in Sec. IV, conclusions are stated and finally, appendices give more details about longer derivations.

II. DERIVATION

A. Preliminaries

The starting point is the extended energy principle, which describes the system as if consisting of a body of plasma, separated from a conducting wall by a vacuum layer.¹⁸ The energy of the whole system, comprised of kinetic energy and potential energy of the plasma, a possible edge current at the plasma surface and the magnetic energy of the surrounding vacuum, is perturbed linearly and the eigenvalues corresponding to this perturbation can be found from the stationary values of the *Rayleigh quotient*:

$$\Lambda[\xi, \mathbf{Q}_v] \equiv \frac{\delta W[\xi, \mathbf{Q}_v]}{K[\xi]} \equiv \frac{\delta W_p[\xi] + \delta W_s[\xi_n] + \delta W_v[\mathbf{Q}_v]}{\frac{1}{2} \int_p \rho |\xi|^2 d\mathbf{r}}. \quad (1)$$

The different terms are given by¹

$$\begin{cases} \delta W_F(\xi) = \frac{1}{2} \int_p d\mathbf{r} \left[\frac{|\mathbf{Q}|^2}{\mu_0} - \xi^* \cdot \mathbf{j} \times \mathbf{Q} + \gamma p |\nabla \cdot \xi|^2 + (\xi \cdot \nabla p) \nabla \cdot \xi^* \right] \\ \delta W_s(\xi_n) = \frac{1}{2} \int_s dS \left[\mathbf{n} \cdot \xi|^2 \mathbf{n} \cdot \left[\nabla \left(\mu_0 p + \frac{B^2}{2} \right) \right] \right]_s \\ \delta W_v(\mathbf{Q}_v) = \frac{1}{2} \int_v d\mathbf{r} \left[\frac{|\mathbf{Q}_v|^2}{\mu_0} \right], \end{cases} \quad (2)$$

where $[\cdot]$ denotes a jump and ξ and \mathbf{Q}_v are the plasma displacement and the vacuum magnetic field perturbation, which have to satisfy only the *essential boundary conditions*

$$\begin{cases} \xi \text{ regular} & (\text{on } V) \\ \mathbf{n} \cdot \nabla \times (\xi \times \mathbf{B}_v) = \mathbf{n} \cdot \mathbf{Q}_v & (\text{on } S) \\ \mathbf{n} \cdot \mathbf{Q}_v = 0 & (\text{on exterior wall } W_v). \end{cases} \quad (3)$$

$\delta \mathbf{B} = \mathbf{Q} = \nabla \times (\xi \times \mathbf{B})$ is the perturbation of the plasma magnetic field and all the other symbols have their usual meaning.

For the plasma potential energy, an equivalent form¹⁹ is used

$$\delta W_F = \frac{1}{2} \int d\mathbf{r} \left[\frac{1}{\mu_0} |\bar{\mathbf{Q}}|^2 + \gamma p |\nabla \cdot \xi|^2 - 2(\xi \cdot \nabla p)(\kappa \cdot \xi^*) - \sigma(\xi^* \times \mathbf{B}) \cdot \bar{\mathbf{Q}} \right], \quad (4)$$

where $\kappa = \hat{\mathbf{b}} \cdot \nabla \hat{\mathbf{b}} = \frac{1}{B^2} \nabla_{\perp} \left(\mu_0 p + \frac{B^2}{2} \right)$ is the curvature, $\sigma \equiv \frac{j_{\parallel}}{B}$ is proportional to the parallel current, and $\bar{\mathbf{Q}}$ is defined as follows:

$$\bar{\mathbf{Q}} = \mathbf{Q} - \mathbf{B} \frac{\mu_0 \xi \cdot \nabla p}{B^2} = \mathbf{Q}_{\perp} - \mathbf{B} [\nabla \cdot \xi_{\perp} + 2\xi_{\perp} \cdot \kappa]. \quad (5)$$

In Eq. (4), the first term can be identified as the stabilizing term due to the perturbation of the magnetic field and the second one due to the perturbation of the plasma. The other two terms show the main driving terms for instabilities, due to the pressure gradient and the parallel current, as discussed in Sec. I.

B. Plasma perturbation and other quantities

In what follows, the same flux coordinates (ψ, θ, ζ) as in Ref. 20 are used:

$$\mathbf{B} = \nabla \zeta \times \nabla \psi + q(\psi) \nabla \psi \times \nabla \theta, \quad (6)$$

which, by defining the field line label $\alpha = \zeta - q(\psi)\theta$, can be brought into Clebsch form in the new (α, ψ, θ) coordinate system

$$\mathbf{B} = \nabla\alpha \times \nabla\psi, \quad (7)$$

where the Jacobian $\mathcal{J}(\alpha, \psi, \theta)$ is identical to the Jacobian in the flux coordinates $\mathcal{J}(\psi, \theta, \zeta)$. In this coordinate system, the parallel derivative reduces to $\mathbf{B} \cdot \nabla = \frac{1}{\mathcal{J}} \frac{\partial}{\partial \theta}$. Note that θ has lost its immediate poloidal significance and now rather means ‘‘along the magnetic field line.’’

In the spirit of Ref. 19 (Eq. (A6)), the plasma perturbation ξ is decomposed in a normal, a geodesic and a parallel component

$$\xi = X \frac{\nabla\psi}{|\nabla\psi|^2} + U \frac{\nabla\psi \times \mathbf{B}}{B^2} + W\mathbf{B}. \quad (8)$$

Employing this, the three components of $\bar{\mathbf{Q}}$, defined in Eq. (5), are given by

$$\begin{cases} \nabla\psi \cdot \bar{\mathbf{Q}} = \frac{1}{\mathcal{J}} \frac{\partial X}{\partial \theta} \\ \frac{\nabla\psi \times \mathbf{B}}{|\nabla\psi|^2} \cdot \bar{\mathbf{Q}} = \frac{1}{\mathcal{J}} \frac{\partial U}{\partial \theta} - SX \\ \mathbf{B} \cdot \bar{\mathbf{Q}} = -B^2 [\nabla \cdot \xi_{\perp} + 2\xi \cdot \kappa] \end{cases} \quad (9)$$

with the total (or local) shear S (Ref. 19) in the (α, ψ, θ) coordinate system

$$\begin{aligned} S &= -\frac{\nabla\psi \times \mathbf{B}}{|\nabla\psi|^2} \cdot \nabla \times \left(\frac{\nabla\psi \times \mathbf{B}}{|\nabla\psi|^2} \right) \\ &= -\frac{1}{\mathcal{J}} \frac{\partial \Theta^{\alpha}}{\partial \theta}, \end{aligned} \quad (10)$$

where $B_i = \mathbf{B} \cdot \mathbf{e}_i$ and $\Theta^i = \frac{\nabla\psi}{|\nabla\psi|^2} \cdot \nabla u^i$, with u^i one of the coordinates (ψ, θ, ζ) .

The curvature lacks a parallel component and, aiming for later compactness of results, the normal and geodesic components are defined as follows:

$$\begin{cases} \kappa_n = \frac{\nabla\psi}{|\nabla\psi|^2} \cdot \kappa = \frac{\nabla\psi}{|\nabla\psi|^2 B^2} \cdot \nabla \left(\mu_0 p + \frac{B^2}{2} \right) \\ \kappa_g = \frac{\nabla\psi \times \mathbf{B}}{B^2} \cdot \kappa = -\frac{1}{2p'} \frac{1}{\mathcal{J}} \frac{\partial \sigma}{\partial \theta}, \end{cases} \quad (11)$$

with $\sigma = \frac{\mathbf{B}}{B^2} \cdot \frac{\nabla \times \mathbf{B}}{\mu_0}$ proportional to the parallel current. Use is made of the fact that the current is divergence-free, implying

$$\nabla \cdot (\mathbf{B}\sigma) - \frac{2}{B^4} \nabla \left(\frac{B^2}{2} \right) \cdot \mathbf{B} \times \nabla p = 0. \quad (12)$$

C. Fourier representation of the perturbation

As mentioned in Sec. I, the modes considered in this work are intermediate to high n in nature. More specifically, this means that these modes are assumed to have a spectral

content that is much higher than the spectral content of the equilibrium quantities. This condition is used further on to make key simplifications.

In this work, a Fourier representation is used, of which the advantages are, on the one hand, that the periodicity constraints that the modes have to comply with are inherently satisfied, and, on the other hand, that the separation of spectra of the equilibrium and the perturbation can be performed mathematically. Furthermore, a Fourier representation does not fail near the plasma edge, as is the case for the higher orders of theory using the ballooning representation, frequently used in theoretical studies.^{6,21}

To avoid large stabilization of the plasma potential energy due to excitation of Alfvén and fast magnetosonic waves (the term containing $\bar{\mathbf{Q}}$ in Eq. (4)), the allowable perturbations have to approximately follow the magnetic field and thus have a *fluted shape*, similarly to the case of normal ballooning modes. Mathematically, this translates in the condition that the parallel derivative be of order 1 and thus

$$\frac{\partial}{\partial \theta} \sim \mathcal{O}(1). \quad (13)$$

This reduces the order of the normal and geodesic components of $\bar{\mathbf{Q}}$ to $\mathcal{O}(1)$ and the only remaining term of order $\mathcal{O}(\epsilon^{-1})$ is $\nabla \cdot \xi_{\perp}$, with ϵ a small parameter that will be defined later. Clearly, not both the derivatives in α and ψ can be chosen of order $\mathcal{O}(1)$, as this would prevent the perturbations from being localized at all. However, their combination in the divergence can indeed be of order $\mathcal{O}(1)$.

Subsequently, the stabilizing term due to sound waves that compress the plasma (the term containing $\nabla \cdot \xi$ in Eq. (4)) is assumed to be minimized to zero by correctly adjusting the parallel component of the perturbation to cancel out the contribution $\nabla \cdot \xi_{\perp}$ due to the perpendicular components (all of order $\mathcal{O}(1)$), though strictly speaking there exist theoretical cases where this is not possible, such as the Z-pinch.²² Thus, the plasma is assumed to be incompressible, suppressing the stabilizing sound waves.

To derive the corresponding criteria relating the two components X and U of ξ_{\perp} , in the (ψ, θ, ζ) coordinate system, the Fourier representation in the variables $\epsilon^{-1}\alpha$ and $\epsilon^{-1}\theta$ is presented, with n the toroidal and m the poloidal mode number

$$\begin{cases} X(\psi, \epsilon^{-1}\theta, \epsilon^{-1}\zeta) = \sum_{m,n} \hat{X}_{m,n}(\psi) e^{i[n\zeta - m\theta]} \\ U(\psi, \epsilon^{-1}\theta, \epsilon^{-1}\zeta|\theta, \zeta) = \sum_{m,n} \hat{U}_{m,n}(\psi|\theta, \zeta) e^{i[n\zeta - m\theta]}, \end{cases} \quad (14)$$

where the notation $(\psi, \epsilon^{-1}\theta, \epsilon^{-1}\zeta|\theta, \zeta)$ means that an additional periodic slow variation of the Fourier amplitude $U_{m,n}$ is allowed, as is customary in *multiple-scale analysis*.²³ It will be seen that this is necessary to cancel secular terms that will appear to ultimately yield a solution that is indeed periodic.

Transforming to the (α, ψ, θ) coordinate system, yields

$$e^{i[n\zeta - m\theta]} \rightarrow e^{i[n\alpha + (nq - m)\theta]}, \quad (15)$$

which means that the condition that the parallel derivatives be of order $\mathcal{O}(1)$ reduces to

$$nq - m \sim \mathcal{O}(1), \tag{16}$$

with q the safety factor.

This has the consequence that the perturbations, though with both $m \sim \mathcal{O}(\epsilon^{-1})$ and $n \sim \mathcal{O}(\epsilon^{-1})$, lie clustered around the line with slope q , as seen in Figure 1, which represents the separation between the spectral content of the equilibrium quantities and the perturbation. This anisotropy has an important implication: The modes do not couple for

$$\begin{aligned} & \sum_{m,n} \left[\int d\theta \int d\alpha A(\alpha, \psi, \theta) e^{i[n-n']\alpha} e^{i[(nq-m)-(n'q-m')]\theta} \right] X_{m,n} X_{m',n'}^* \\ &= \sum_{m,n} \left[\int d\theta \left[\int d\alpha A(\alpha, \psi, \theta) e^{i[n-n']\alpha} \right] e^{i[(nq-m)-(n'q-m')]\theta} \right] X_{m,n} X_{m',n'}^* \\ &\approx \frac{1}{2\pi} \sum_{m,n} \left[\int d\theta A(\alpha, \psi, \theta) \delta_n^{n'} e^{i[(nq-m)-(n'q-m')]\theta} \right] X_{m,n} X_{m',n'}^* \\ &\approx \frac{1}{2\pi} \sum_m \left[\int d\theta A(\alpha, \psi, \theta) e^{i(m'-m)\theta} \right] X_m X_{m'}^* |_{n=n'}, \end{aligned} \tag{17}$$

implying that, though the equilibrium quantities vary across the magnetic field lines, in the coordinate α , they are quasi-constant in the $n\alpha$ scales on which the perturbations vary, effectively removing A from the integral in α . The same cannot be done for the integral along the magnetic field lines in θ , since the perturbations vary as slowly as the equilibrium quantities due to their flutedness.

Note that the integral along θ is a field-line average: *Toroidal information about the equilibrium is preserved*, since the magnetic field line varies toroidally. This in contrast to the axisymmetric case where the line average can be reduced to an average in the poloidal angle, as in Ref. 12.

Therefore, ultimately, the Fourier representations for X and U used are

$$\begin{cases} X = \sum_m \hat{X}_m(\psi) e^{i[n\alpha + (nq-m)\theta]} \\ U = \sum_m \hat{U}_m(\psi|\alpha, \theta) e^{i[n\alpha + (nq-m)\theta]}, \end{cases} \tag{18}$$

with the exponents containing both terms of order $\mathcal{O}(1)$ and of order $\mathcal{O}(n)$ with ϵ from now on chosen to be equal to n^{-1} .

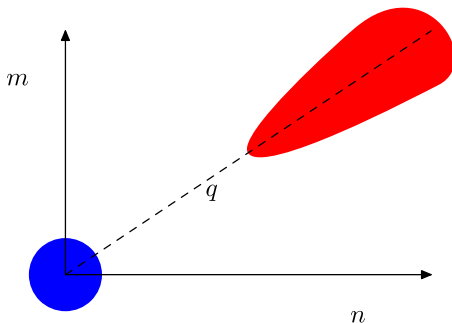


FIG. 1. A sketch of the assumed spectra of the equilibrium quantities (blue) and the perturbation (red, hatched). The horizontal axis indicates the toroidal wave number n and the vertical axis the poloidal wave number m .

different magnetic field lines (represented by the coordinate α), but only along magnetic field lines (represented by θ), so the double summation reduces to a single summation over m .

This result can be indicated symbolically by considering the following representation for the plasma potential energy that explicitly shows the coupling between a mode with mode numbers n and m and a mode with n' and m' , and where A represents equilibrium quantities

D. Minimizing plasma perturbation

In a first step, the fast variation across the magnetic field lines, in the coordinate $n\alpha$, is introduced by inserting only the fast part of the full Fourier representations of Eq. (18)

$$\begin{cases} X = \hat{X}(\psi, \theta) e^{in\alpha} \\ U = \hat{U}(\psi, \theta|\alpha, \theta) e^{in\alpha}, \end{cases} \tag{19}$$

into the condition $\nabla \cdot \xi_{\perp} \sim \mathcal{O}(1)$. To this end, an ordering technique for the normal perturbation X is applied as follows:

$$X = X^{(0)} + X^{(1)} + \dots, \tag{20}$$

with $|X^{(k)}|/|X^{(k+1)}| \sim \mathcal{O}(n)$. Doing the same for the other components, a condition for the first orders $X^{(0)}$ and $U^{(0)}$ is derived

$$\hat{U}^{(0)} = \left(-\Theta^{\alpha} + \frac{i}{n} \left(\frac{\partial}{\partial \psi} + \Theta^{\theta} \frac{\partial}{\partial \theta} \right) \right) \hat{X}^{(0)}. \tag{21}$$

Note that the θ component has been included for the term in X , even though it is formally of lower order than the other two. This is done in hindsight by realizing that it is the most convenient way for the geodesic perturbation to be periodic (see further below), simplifying the two-scale analysis. The same result could be obtained by considering the problem in the unmodified flux coordinates (ψ, θ, ζ) , but would require a little bit more work.

Subsequently, the second order can be minimized as well making use of the first order result. Collecting terms in the divergence and combining them with the curvature term yields an expression correct up to order $\sim \mathcal{O}(n^{-1})$

$$0 = \left(in\Theta^{\alpha} + \frac{\partial}{\partial \psi} + \Theta^{\theta} \frac{\partial}{\partial \theta} \right) \hat{X} + in\hat{U} + \hat{Q}(\hat{X}), \tag{22}$$

where the second-order operator \hat{Q} is defined as

$$\begin{aligned} \hat{Q}(\beta) = & \left[\frac{1}{\mathcal{J}} \frac{\partial}{\partial u^i} (\mathcal{J} \Theta^i) + 2\kappa_n \right] \beta \\ & + \left[2\kappa_g + \frac{1}{\mathcal{J}} \frac{\partial \mathcal{J}}{\partial \alpha} - \frac{1}{\mathcal{J}} \frac{\partial}{\partial \theta} \left(\frac{B_x}{B^2} \right) - \frac{1}{\mathcal{J} B^2} \frac{\partial}{\partial \theta} + \frac{\partial}{\partial \alpha} \right] \\ & \times \left[\left(-\Theta^\alpha + \frac{i}{n} \left(\frac{\partial}{\partial \psi} + \Theta^\theta \frac{\partial}{\partial \theta} \right) \right) \beta \right]. \end{aligned} \quad (23)$$

This eliminates the parallel component of the magnetic terms and reduces the entire stabilizing magnetic term to order $\sim \mathcal{O}(1)$.

In a second step, the previous expression for Q is now simplified by inserting the remainder of the Fourier representation for the coordinate $(nq - m)\theta$, the slow coordinate along the magnetic field

$$\begin{cases} \hat{X} = \sum_m \hat{X}_m(\psi) e^{i(nq-m)\theta} \\ \hat{U} = \sum_m \hat{U}_m(\psi|\alpha, \theta) e^{i(nq-m)\theta}. \end{cases} \quad (24)$$

For ease of notation, in what follows, the hat is left out and it is to be understood implicitly that Fourier modes are treated. In any case, the presence of a subscript m denotes a (complete) Fourier mode.

Using above, the condition (22) becomes

$$U_m = \left(-\Theta^\zeta + \frac{m}{n} \Theta^\theta + \frac{i}{n} \frac{\partial}{\partial \psi} \right) X_m + \frac{i}{n} Q_m(X_m), \quad (25)$$

relating U_m to X_m , with $\Theta^\zeta \equiv \Theta^\alpha + q'\theta + \Theta^\theta q$ and

$$Q_m(X_m) = \left(Q_m^0 + Q_m^1 \frac{i}{n} \frac{d}{d\psi} \right) (X_m), \quad (26)$$

where Q_m^0 and Q_m^1 only depend on equilibrium quantities. They are calculated in Appendix A

$$\begin{cases} Q_m^0 = \frac{B_x q' + \mathcal{J} \mu_0 p'}{B_\theta} + \left(-\Theta^\zeta + \Theta^\theta \frac{m}{n} \right) Q_m^1 \\ \quad + \frac{nq - m}{n} \frac{\mathcal{J} \mathbf{B} \cdot \nabla \psi \times \nabla \Theta^\theta}{B_\theta} \\ Q_m^1 = -i(nq - m) \frac{B_x}{B_\theta}. \end{cases} \quad (27)$$

Note that the term proportional to Q_m in Eq. (25) is an order of magnitude smaller than the other terms and that U_m indeed has a slow-varying component in the coordinates α and θ . Also note that the relative strength of the dependence on ψ is not important. Inserting the expression thus obtained for the modes U_m into Eq. (4) then yields an expression for the plasma potential energy, as a function of the normal displacement X_m only, correct up to second order in n .

Summarizing, by first requiring the entire stabilizing magnetic energy to be finite and of order $\mathcal{O}(1)$, leading to fluted modes, and subsequently minimizing the magnetic compressional energy to zero, above expression for the geodesic component of the Fourier modes U_m was derived,

expressed as a function of X_m (Eq. (25)). This allowed for the complete description of the plasma potential energy as a function of the normal component X_m .

Finally, mixing the different orders of the terms, this expression can be split into a linear part and a part corresponding to the first derivative

$$U_m = \left(U_m^0 + U_m^1 \frac{i}{n} \frac{\partial}{\partial \psi} \right) (X_m), \quad (28)$$

with:

$$\begin{cases} U_m^0 = -\Theta^\zeta + \Theta^\theta \frac{m}{n} + \frac{i}{n} Q_m^0 \\ U_m^1 = 1 + \frac{i}{n} Q_m^1, \end{cases} \quad (29)$$

where Q_m^0 and Q_m^1 are defined in Eq. (27). U_m can thus be seen as a linear differential operator, acting on the modes of the normal perturbation. In what follows, it is found useful to assign a symbol to the parallel derivative of U in θ , which can be written out compactly

$$\frac{\partial U_m}{\partial \theta} = \left(DU_m^0 + DU_m^1 \frac{i}{n} \frac{\partial}{\partial \psi} \right) (X_m), \quad (30)$$

with

$$\begin{cases} DU_m^0 = i(nq - m) U_m^0 + \frac{\partial U_m^0}{\partial \theta} \\ DU_m^1 = i(nq - m) U_m^1 + \frac{\partial U_m^1}{\partial \theta}. \end{cases} \quad (31)$$

E. Minimization of plasma potential energy

To obtain the expression for the plasma potential energy, it is useful to define the adjoint of the linear operator U_k^*

$$\langle U_k(\alpha), \beta \rangle_\psi = \langle \alpha, U_k^T(\beta) \rangle - \left[\mathcal{J} \frac{i}{n} U_k^{1*} \alpha^* \beta \right]_{\psi_a}^{\psi_s}, \quad (32)$$

where the boundary term, with ψ_a a flux surface deep inside the plasma and ψ_s at the plasma edge, arises from the fact that external modes are considered, which do not necessarily vanish at the limits of integration. The inner product is defined as

$$\langle \alpha, \beta \rangle_\psi = \int_{\psi_a}^{\psi_s} \mathcal{J} \alpha^* \beta d\psi, \quad (33)$$

and the operator U_k^T as

$$U_k^T(\beta) = \left(U_k^{T,0} + U_k^{T,1} \frac{i}{n} \frac{\partial}{\partial \psi} \right) \beta, \quad (34)$$

with

$$\begin{cases} U_k^{T,0} = U_k^{0*} + \frac{1}{\mathcal{J} n} \frac{\partial}{\partial \psi} (U_k^{1*} \mathcal{J}) \\ U_k^{T,1} = U_k^{1*}, \end{cases} \quad (35)$$

and equivalently for DU from Eq. (30).

Now, the series of Eq. (18) is introduced into the plasma potential energy, given by Eq. (4), making use of the above expression of the adjoint operators U_k^T and DU_k^T . In Appendix B, it is shown that this reduces to a volume integral with three types of terms concerning the coupling of the modes m and k ($\equiv m'$): Those proportional to the amplitude

of the mode X_m , those proportional to the first derivative in ψ of X_m , and those proportional to the second, and all terms also proportional to the amplitude X_k^* of mode k . This is accompanied by a surface integral, with two types of terms. The expression for the plasma potential energy then has the form:

$$\frac{1}{2} \sum_{k,m} \int_{\psi_a}^{\psi_s} d\psi \left[\int d\theta \mathcal{J} X_k^* e^{i(k-m)\theta} \left\{ PV_{k,m}^0 + PV_{k,m}^1 \left(\frac{i}{n} \right) \frac{d}{d\psi} + PV_{k,m}^2 \left(\frac{i}{n} \right)^2 \frac{d^2}{d\psi^2} \right\} X_m \right], \tag{36}$$

along with a surface term

$$\frac{1}{2} \sum_{k,m} \int d\theta \mathcal{J} X_k^* e^{i(k-m)\theta} \left\{ PS_{k,m}^0 + PS_{k,m}^1 \left(\frac{i}{n} \right) \frac{d}{d\psi} \right\} X_m |_{\psi_s}, \tag{37}$$

with the coefficients $PV_{k,m}^i$ and $PS_{k,m}^i$ given by

$$\begin{cases} PV_{k,m}^0 = \widetilde{P}V_{k,m}^0 + \frac{1}{\mathcal{J}} \frac{i}{n} \frac{\partial}{\partial \psi} \left(\mathcal{J} \widetilde{P}V_{m,k}^{1*} \right), & PS_{k,m}^0 = -\frac{i}{n} \widetilde{P}V_{m,k}^{1*}, \\ PV_{k,m}^1 = \left(\widetilde{P}V_{k,m}^1 + \widetilde{P}V_{m,k}^{1*} \right) + \frac{1}{\mathcal{J}} \frac{i}{n} \frac{\partial}{\partial \psi} \left(\mathcal{J} \widetilde{P}V_{k,m}^2 \right), & PS_{k,m}^1 = -\frac{i}{n} \widetilde{P}V_{k,m}^2, \\ PV_{k,m}^2 = \widetilde{P}V_{k,m}^2, \end{cases} \tag{38}$$

with

$$\begin{cases} \widetilde{P}V_{k,m}^0 = \frac{1}{\mu_0} \frac{|\nabla\psi|^2}{\mathcal{J}^2 B^2} (DU_k^{0*} - \mathcal{J}S)(DU_m^0 - \mathcal{J}S) + \frac{1}{\mathcal{J}} \frac{\partial \sigma}{\partial \theta} (U_k^{0*} + U_m^0) + S\sigma \\ \quad + \frac{\sigma}{\mathcal{J}} \left(i(nq - m)U_k^{0*} - i(nq - k)U_m^0 \right) + \frac{1}{\mu_0} \frac{(nq - k)(nq - m)}{\mathcal{J}^2 |\nabla\psi|^2} - 2p' \kappa_n \\ \widetilde{P}V_{k,m}^1 = \frac{1}{\mu_0} \frac{|\nabla\psi|^2}{\mathcal{J}^2 B^2} (DU_k^{0*} - \mathcal{J}S)DU_m^1 + \frac{U_m^1}{\mathcal{J}} \frac{\partial \sigma}{\partial \theta} - \sigma \frac{U_m^1}{\mathcal{J}} i(nq - k) \\ \widetilde{P}V_{k,m}^2 = \frac{1}{\mu_0} \frac{|\nabla\psi|^2}{\mathcal{J}^2 B^2} DU_m^1 DU_k^{1*}. \end{cases} \tag{39}$$

The two derivative terms in $PV_{k,m}^i$ are crucial for Hermiticity of the plasma potential energy. This can best be seen by inserting Eqs. (38) and (39) into Eq. (36) and cancelling the surface terms from Eq. (37). The integrand of Eq. (36), including the double summation, then can be written in tensorial notation

$$(\mathbf{X}^*)^T \mathbf{P} \mathbf{X}, \tag{40}$$

where a factor $\mathcal{J}/2$ has been left out, with $\mathbf{X} = (X_m e^{-im\theta})^T$ and the elements of the tensor \mathbf{P} given by

$$\begin{aligned} P_{k,m} &= \widetilde{P}V_{k,m}^0 - \frac{i}{n} \frac{\partial}{\partial \psi} \widetilde{P}V_{m,k}^{1*} + \widetilde{P}V_{k,m}^1 \frac{i}{n} \frac{\partial}{\partial \psi} \\ &\quad - \frac{i}{n} \frac{\partial}{\partial \psi} \widetilde{P}V_{k,m}^2 \frac{i}{n} \frac{\partial}{\partial \psi}, \end{aligned} \tag{41}$$

which are indeed Hermitian. The arrows indicate whether the derivatives act on the right or on the left.

F. Edge and vacuum energy

The edge term, given in Eq. (2), is associated with a sheet current \mathbf{J}_s running on the edge of the plasma that provokes a discontinuity in the magnetic field on either side of the last flux surface of the plasma and is given by applying Ampère's law

$$\mathbf{J}_s = \hat{\mathbf{n}} \times [\mathbf{B}]. \tag{42}$$

Though a theoretical possibility, in practice, an equilibrium edge current is unusual and therefore left out.²⁴ In addition, by considering the essential boundary conditions of Eq. (3), it can be seen that the inclusion of an equilibrium edge current would lead to a highly stabilizing vacuum

$$\mathbf{Q}_v \cdot \nabla \psi = \mathbf{B}_v \cdot \nabla X \quad \text{at } s. \quad (43)$$

Indeed, the derivative of X in the direction of \mathbf{B}_v is of order $\mathcal{O}(n)$ if $\mathbf{B} \neq \mathbf{B}_v$, which would imply that the vacuum perturbation \mathbf{Q}_v be of that order as well, leading to a large vacuum stabilization. This is to be avoided.

The vacuum energy, also given in Eq. (2), is always stabilizing and should be minimized while respecting the essential boundary conditions of Eq. (3). Since the vacuum is current-free, the vacuum magnetic perturbation \mathbf{Q}_v satisfies

$$\nabla \cdot \mathbf{Q}_v = \nabla \times \mathbf{Q}_v = 0, \quad (44)$$

which implies that it can be represented by a scalar potential ϕ that has to obey Laplace's equation:

$$\nabla^2 \phi = 0, \quad (45)$$

connected to the plasma by the essential boundary condition and assumed to vanish at infinity:

$$\nabla \psi \cdot \nabla \phi = \begin{cases} \mathbf{B} \cdot \nabla X & \text{at } s \\ 0 & \text{at } w. \end{cases} \quad (46)$$

Then, the vacuum energy term can be rewritten as

$$\begin{aligned} \delta W_v &= \frac{1}{2\mu_0} \int_v \mathbf{dr} [\nabla \cdot (\phi \nabla \phi^*)] = \frac{1}{2\mu_0} \int_{\partial v} \mathbf{dS} \cdot (\nabla \phi^*) \phi \\ &= -\frac{1}{2\mu_0} \int_s \mathcal{J}(\mathbf{B} \cdot \nabla X^*) \phi \, d\theta \, d\alpha, \end{aligned} \quad (47)$$

where the negative sign is due to the difference between the definition of the outward normal of the plasma volume and the direction of increasing magnetic flux. The perturbation is assumed to vanish at the surrounding wall, located far away from the plasma, which is justified since peeling-ballooning perturbations are assumed to be radially localized to some extent. ϕ is to be solved with Laplace's equation as a function of the plasma perturbation X at the edge.

This is done conveniently using Green's method, based on Green's second identity:^{24,25}

$$\nabla \cdot (a \nabla b) = a \nabla^2 b + \nabla a \cdot \nabla b, \quad (48)$$

which, upon interchanging a and b , taking the difference between both equations and integrating over a volume yields:

$$\int_v (a \nabla^2 b - b \nabla^2 a) \, dV = \int_{\partial v} (a \nabla b - b \nabla a) \cdot \mathbf{dS}. \quad (49)$$

This equation is used by setting $a = \phi(\mathbf{r})$ and $b = G_N(\mathbf{r}, \mathbf{r}') = \frac{1}{|\mathbf{r} - \mathbf{r}'|} + F(\mathbf{r}, \mathbf{r}')$, a modified Green's function for Neumann boundary conditions²⁶ for the Laplacian in three dimensions, with $\nabla^2 G = -\delta(\mathbf{r} - \mathbf{r}')$ and F a function that is symmetric in its arguments and satisfies

$$\begin{cases} \nabla^2 F(\mathbf{r}, \mathbf{r}') = 0 \\ \nabla \psi \cdot \nabla G_N = -\frac{4\pi}{\partial v}, \end{cases} \quad (50)$$

with ∂v the total surface surrounding the volume. Choosing this equal to the vacuum volume and evaluating at a point in the plasma edge, this yields an expression for the vacuum potential²⁷

$$\phi(\mathbf{r}) = \langle \phi \rangle + \iint_{\partial v} G_N(\mathbf{r}, \mathbf{r}') \nabla' \phi(\mathbf{r}') \cdot \mathbf{dS}', \quad (51)$$

where $\langle \phi \rangle$ is the average value of the potential over the whole surface.

Since the perturbation is assumed to vanish at the surrounding wall, the more complicated treatment of low n codes such as vacuum²⁵ that take into account the image currents in the surrounding wall, is not needed here. So, upon introducing the boundary conditions from Eq. (46) and realizing that the average potential goes to zero due to the surrounding wall, assumed to be at infinity, Eq. (51) becomes

$$\phi(\mathbf{r}) = - \iint_s G_N(\mathbf{r}, \mathbf{r}') \mathcal{J} \mathbf{B}(\mathbf{r}') \cdot \nabla' X(\psi) \, d\alpha' \, d\theta'. \quad (52)$$

Inserting this relation between the potential and the plasma perturbation $X_{m,s}(\psi)$ at the edge of the plasma into Eq. (47) yields

$$\delta W_v = \frac{1}{2} \sum_{k,m} X_k^* \left[\iint_s \mathcal{J} \, d\theta \, d\alpha \right] \left[\iint_s \mathcal{J} \, d\theta' \, d\alpha' \, V S_{k,m} \right] X_m, \quad (53)$$

with the Hermitian coefficients $V S_{k,m}$ given by

$$V S_{k,m} = \frac{1}{\mu_0} \frac{G_N(\mathbf{r}, \mathbf{r}')}{\mathcal{J}^2} e^{i[n(\alpha' - \alpha) + (nq - m)\theta' - (nq - k)\theta]} (nq - m)(nq - k). \quad (54)$$

G. Kinetic energy

Finally, the last ingredient in the extended spectral variational principle described in Subsection II A is the plasma kinetic energy, given by

$$K[\xi] = \frac{\omega^2}{2} \int_p \rho |\xi|^2 \, d\mathbf{r}, \quad (55)$$

where ρ is the density of the plasma.

Now, as stated above, in Subsection II D, the minimization of the plasma compressional energy to zero by adjusting the parallel component is relatively simple, and unaffected by the kinetic energy if the kinetic energy of the parallel component is neglected. Not doing this would raise the complexity of the problem, as the number of equations that has to be solved would double. As the applicability and accuracy of the parallel dynamics of the basic ideal MHD theory are questionable, this is not a major simplification and, in any case, it represents a worst-case scenario since the plasma sound waves are stabilizing.²²

Since in the (perpendicular) plasma kinetic energy no derivatives of the perturbation appear, these terms do not influence the minimization of the magnetic compression term of the plasma potential energy performed in Subsection II D and the results obtained there relating the geodesic perturbation U to the normal perturbation X are introduced in above formula for the plasma kinetic energy

$$\begin{aligned}
K_{\perp} &= \frac{\omega^2}{2} \int_{\text{p}} \mathbf{d}\mathbf{r} \rho \left[\frac{1}{|\nabla\psi|^2} |X|^2 + \frac{|\nabla\psi|^2}{B^2} |U|^2 \right] \\
&= \frac{\omega^2}{2} \int_{\text{p}} \mathbf{d}\mathbf{r} \rho \sum_{k,m} e^{i(k-m)\theta} \left[\frac{1}{|\nabla\psi|^2} X_k^* X_m + \frac{|\nabla\psi|^2}{B^2} U_k^*(X_k^*) U_m(X_m) \right] \\
&= \frac{\omega^2}{2} \int_{\text{p}} \mathbf{d}\mathbf{r} \sum_{k,m} X_k^* e^{i(k-m)\theta} \left[\frac{\rho}{|\nabla\psi|^2} + U_k^T \frac{\rho |\nabla\psi|^2}{B^2} U_m \right] (X_m), \tag{56}
\end{aligned}$$

where the operators work on everything to their right, resulting in volume and surface coefficients equivalent to the ones used Eqs. (36) and (37)

$$\begin{cases} \widetilde{KV}_{k,m}^0 = \frac{\rho}{|\nabla\psi|^2} + \frac{|\nabla\psi|^2}{B^2} U_k^{0*} U_m^0 \rho \\ \widetilde{KV}_{k,m}^1 = \frac{|\nabla\psi|^2}{B^2} U_k^{0*} U_m^1 \rho \\ \widetilde{KV}_{k,m}^2 = \frac{|\nabla\psi|^2}{B^2} U_k^{1*} U_m^1 \rho. \end{cases} \tag{57}$$

Using the same arguments as in Subsection II E, the integrand of the plasma kinetic energy integral can be written in a Hermitian form equivalent to Eq. (40).

III. DISCUSSION

In the previous section, expressions were found for the potential energy due to the plasma, which was described by three volume coefficients $PV_{k,m}^i$ and two surface coefficients $PS_{k,m}^i$, the plasma kinetic energy, described by $KV_{k,m}^0$ and $KS_{k,m}^0$, and the potential energy due to the edge and vacuum, of which the former is neglected and the latter is described by $VS_{k,m}$.

By taking the Euler minimization with respect to each of the M amplitudes of the Fourier modes X_k^* , an equation in the M unknowns X_m is obtained. The result can be summarized by the following equation that has to be solved for every field line:

$$\begin{aligned}
\sum_m \left\{ \langle e^{i(k-m)\theta} V_{k,m}^0 \rangle_{\theta} + \langle e^{i(k-m)\theta} V_{k,m}^1 \rangle_{\theta} \left(\frac{i}{n} \right) \frac{d}{d\psi} \right. \\
\left. + \langle e^{i(k-m)\theta} V_{k,m}^2 \rangle_{\theta} \left(\frac{i}{n} \right)^2 \frac{d^2}{d\psi^2} \right\} X_m = 0, \tag{58}
\end{aligned}$$

for $k = m_0 \dots m_0 + M$ and with the field-line average $\langle \cdot \rangle_{\theta}$ defined as:

$$\langle A \rangle_{\theta} = \int_{-\infty}^{\infty} \mathcal{J} A \, d\theta, \tag{59}$$

with the coefficients $V_{k,m}^i$ given by

$$V_{k,m}^i = PV_{k,m}^i - \omega^2 KV_{k,m}^i, \tag{60}$$

from Eq. (38) and an equivalent for $KV_{k,m}^i$.

The restriction due to the normalization of the plasma kinetic energy using a Lagrange multiplier ω^2 is mathematically equivalent to the minimization of the Rayleigh quotient of Eq. (1) with an eigenvalue ω^2 and the appropriate boundary conditions shown below.²⁷

This is a system of M ordinary differential equations of second degree for the M different amplitudes X_m . Two boundary conditions are needed, the first one being the assumption that the perturbation vanishes deep into the plasma. The second boundary condition comes by minimizing the surface contributions from the plasma potential and kinetic energy and from the vacuum term, which leads to N equations

$$\sum_m \left\{ \langle e^{i(k-m)\theta} S_{k,m}^0 \rangle + \langle e^{i(k-m)\theta} S_{k,m}^1 \rangle \frac{i}{n} \frac{\partial}{\partial \psi} + \delta_{k,m}^{\text{vac}} \right\} X_m = 0, \tag{61}$$

where the surface coefficient $PS_{k,m}$ is given by Eqs. (38) and equivalent for $KS_{k,m}$ and the vacuum term is given by the integrand of Eq. (53). These M equations provide a relation between the plasma perturbation of the M modes at the boundary.

The solution of this system of equations has to be done numerically. This will be the subject of a future paper.

A. Identification of terms

The terms due the plasma potential energy, given by Eq. (38), clearly show the intuitive structure of Eq. (4), where the stabilizing and potentially destabilizing terms can be identified

- The stabilizing magnetic terms, described by $\frac{1}{\mu_0} |\bar{\mathbf{Q}}|^2$, have only a normal and a geodesic component, as the parallel component is minimized to zero. The normal component, reflected in the fifth term of $\widetilde{PV}_{k,m}^0$, relates to $\frac{1}{\mathcal{J}} \frac{\partial X}{\partial \theta}$ of Eq. (9), whereas the geodesic component is reflected in the first terms of $\widetilde{PV}_{k,m}^0$, $\widetilde{PV}_{k,m}^1$, and $\widetilde{PV}_{k,m}^2$ and relates to $\frac{1}{\mathcal{J}} \frac{\partial U}{\partial \theta} - SX$ of Eq. (9).
- The stabilizing plasma compression term is not present as this is minimized to zero by adjusting the parallel component of the perturbation.
- Since the geodesic curvature is related to $\frac{\partial \sigma}{\partial \theta}$ through Eq. (11), the last term of $\widetilde{PV}_{k,m}^0$, along with the part containing the complex conjugate of the second term of $\widetilde{PV}_{k,m}^0$ and the second term of $\widetilde{PV}_{m,k}^{1*}$ represent the destabilizing

term due to the pressure gradient. This is the main driving term of the ballooning instability, $-2(\xi \cdot \nabla p)(\kappa \cdot \xi^*)$.

- Finally, through Eq. (B10), the other part of the second term of $\widetilde{P}\widetilde{V}_{k,m}^0$, the third and fourth term of $\widetilde{P}\widetilde{V}_{k,m}^0$, the second term of $\widetilde{P}\widetilde{V}_{k,m}^1$ and the third terms of $\widetilde{P}\widetilde{V}_{k,m}^1$ and $\widetilde{P}\widetilde{V}_{m,k}^{1*}$ correspond to the destabilizing term due to the parallel current σ . This is the main driving term of the kink instability, $-\sigma(\xi^* \times \mathbf{B}) \cdot \bar{\mathbf{Q}}$.

For the plasma kinetic energy, a similar analysis can be easily made, showing that the first term of $\widetilde{K}\widetilde{V}_{k,m}^0$ corresponds to the normal part and all the rest to the geodesic part. The parallel part was neglected.

B. Axisymmetric approximation

In the axisymmetric approximation, employed in Ref. 12 and subsequent papers, a derivation has been done similar to the one in the work presented here, with the major exception that there it is assumed that the plasma equilibrium and the perturbations have axisymmetric symmetry. This results in simplifications in the derivations, but also limits the applicability of the results.

The axisymmetric results equivalent to Eq. (60) from Ref. 12 are based on the theory derived in Ref. 6. However, the comparison between the results from Ref. 12 and the results from this work, with the axisymmetric approximation inserted, is only feasible experimentally, by actually calculating the energy for certain test cases, because the direct axisymmetric results in Ref. 12 are not written in a compact and clearly self-adjoint form, and could be written in a virtually unlimited number of similar ways.

What is shown here, however, is a demonstration of the agreement between the results from Ref. 6, on which the direct axisymmetric results are based, with Eq. (4), which is the basis of the 3D theory developed here.

First of all, the “straight field line angle” ω of Ref. 12 is identified as the flux coordinate θ_F which is related to

the measure of the length along the magnetic field, since $\mathbf{B} = \frac{1}{\mathcal{J}_F} \mathbf{e}_{\theta_F}$ as seen from Eq. (7). Therefore, the following relations between the flux coordinates and the axisymmetric coordinates:

$$\begin{cases} \alpha_F = \zeta_A - \int^{\zeta_A} \nu \, d\chi \\ \psi_F = \psi_A \\ \theta_F = \frac{1}{q} \int^{\zeta_A} \nu \, d\chi \equiv \omega, \end{cases} \quad (62)$$

to transform from the 3D flux coordinate system $(\alpha_F, \psi_F, \zeta_F)$ used here to the axisymmetric coordinate system $(\psi_A, \chi_A, \zeta_A)$ used in Ref. 6 (with the orientation inverted, consistent with subsequent papers), can be found.

Using this, expression (27) is simplified for the axisymmetric case and inserted into the expression for the minimizing geodesic perturbation U_m from Eq. (25)

$$\begin{cases} U_m^0 = \frac{m}{n} \omega' \left(1 + \frac{nq - mf^2/R^2}{nq} \frac{1}{B^2} \right) \\ \quad + \frac{i}{n} \left(-\frac{mf^2/R^2}{n} \frac{1}{B^2} \frac{1}{\nu} \left(\frac{\nu}{q} \right)' + \frac{1}{\mathcal{J}_A} \frac{\partial \mathcal{J}_A}{\partial \psi} + 2\kappa_n \right) \\ U_m^1 = 1 + \frac{nq - mf^2/R^2}{nq} \frac{1}{B^2}. \end{cases} \quad (63)$$

This expression corresponds to the direct axisymmetric result found in Ref. 6 (Eq. (12), which can be seen by inserting the slow dependence $X = X_m e^{-im\omega}$ and $U = U_m e^{-im\omega}$ (the fast ζ -dependence has already been accounted for) and rewriting it for U_m

$$U_m = \frac{i}{n} \frac{\partial X_m}{\partial \psi} + \frac{m}{n} \omega' X_m + e^{im\omega} \frac{i}{n} Q_{\text{connor}}, \quad (64)$$

with Q_{connor} given at the bottom of the same page. Indeed, this yields

$$\begin{aligned} Q_{\text{connor}} &= \frac{f^2/R^2}{B^2 \nu} \mathcal{J}_A B k_{\parallel} \left(\frac{1}{n} \frac{\partial X}{\partial \psi} \right) + X \left(\frac{1}{\mathcal{J}_A} \frac{\partial \mathcal{J}_A}{\partial \psi} + 2\kappa_n \right) \\ &= \left\{ \frac{f^2/R^2}{B^2} \left[\frac{nq - m}{nq} \frac{\partial}{\partial \psi} - \left(\frac{m}{n} \left(\frac{1}{\nu} \right) \left(\frac{\nu}{q} \right)' + \omega' im \frac{nq - m}{nq} \right) \right] (X_m) + X_m \left(\frac{1}{\mathcal{J}_A} \frac{\partial \mathcal{J}_A}{\partial \psi} + 2\kappa_n \right) \right\} e^{-im\omega}, \end{aligned} \quad (65)$$

which is equivalent to Eq. (63).

Subsequently, inserting the minimized U_m into Eq. (4), assuming axisymmetry and taking the same steps as to get to Eq. (36), inserting fast Fourier modes (Ref. 12, Eq. (1)) could be relatively easily derived, which is the starting point of the theory behind ELITE. Introducing the slow Fourier

modes then leads to the axisymmetric equivalent to Eq. (60). As the original derivation in Ref. 6 was quite cumbersome, this is a useful alternative that also provides deeper physical insight. The derivation has been verified by the first author but, due to lack of space, is only mentioned here, without reproducing it.

These results hint at the correctness of the 3D theory derived here, at least considering the axisymmetric limit as a verification and the necessary Hermiticity. More thorough comparisons will be the subject of future work.

IV. CONCLUSIONS

Intermediate to high linear n modes in full 3D configurations were investigated theoretically using MHD theory. This is of interest because of peeling-ballooning modes, which are thought to play an important role for the cyclic behavior of ELMS in magnetic fusion reactors and could also clarify some of the issues concerning the limits of the high confinement H-mode observed in many of these devices.

The work presented here builds up on the previous theoretical basis in Refs. 12 and 19, which was based in turn on.⁶ The major innovation in this work is that the condition of axisymmetry is relaxed and thus provides results which are more widely applicable than those from previous studies.

Thus, a full 3D treatment of the stability of peeling-ballooning modes with intermediate to high n mode numbers, valid also near the edge of the plasma, was developed making use of a Fourier expansion that included a multiple-scale analysis to separate the spectral content of the equilibrium and the perturbation, based on the extended energy principle first cornered by Ref. 18.

The results of the theoretical investigation of this work are a concise Hermitian set of M second order linear differential equations for M poloidally coupled modes resulting from the energy minimization. These equations have to obey

two boundary conditions each, one of which is the vanishing of the modes deep inside the plasma and the other one is a relation found by minimizing the surface terms of the energy of the plasma and the vacuum. This system of equations has to be solved numerically, which will be the focus of future work.

The 3D equations derived in this study have been applied to the axisymmetric situation and it has been demonstrated that previous results in this approximation can be reproduced, which provides an initial proof of the correctness of the theoretical model developed here. Further simplified verification of the validity of the 3D approach will be carried out when the numerical implementation of the model is developed. Subsequently, the results will be used to investigate various 3D effects, such as toroidal ripple in tokamaks, the behavior of perturbation coils for the control of ELMS, the influence of a TBM module, etc.

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APPENDIX A: CALCULATION OF Q

By using

$$\begin{aligned} & \frac{\partial}{\partial \alpha} \left[\left(-\Theta^\alpha + \frac{i}{n} \left(\frac{\partial}{\partial \psi} + \Theta^\theta \frac{\partial}{\partial \theta} \right) \right) (X_m(\psi) e^{i(nq-m)\theta}) \right] \\ &= \frac{\partial}{\partial \alpha} \left[\left(-\left(\Theta^\alpha + q'\theta + \Theta^\theta \frac{nq-m}{n} \right) + \frac{i}{n} \frac{\partial}{\partial \psi} \right) (X_m(\psi)) \right] e^{i(nq-m)\theta} \\ &= \left[-\frac{\partial \Theta^\alpha}{\partial \alpha} - \frac{\partial \Theta^\theta}{\partial \alpha} \frac{nq-m}{n} \right] X_m(\psi) e^{i(nq-m)\theta}. \end{aligned} \quad (A1)$$

Eq. (23) can be described, upon introducing the slow Fourier modes defined in Eq. (24), by the operators Q_m^0 and Q_m^1 from Subsection II D:

$$\begin{cases} Q_m^0 = \left(\frac{\partial}{\partial \theta} - \frac{nq-m}{n} \frac{\partial}{\partial \alpha} \right) \Theta^\theta + \frac{\Theta^i}{\mathcal{J}} \frac{\partial \mathcal{J}}{\partial u^i} + 2\kappa_n + \frac{B_x}{\mathcal{J}B^2} \frac{\partial}{\partial \theta} \left(\Theta^\zeta - \Theta^\theta \frac{m}{n} \right) + \left(-\Theta^\zeta + \Theta^\theta \frac{m}{n} \right) Q_m^1 \\ Q_m^1 = -i(nq-m) \frac{B_x}{\mathcal{J}B^2} + \frac{1}{\mathcal{J}} \frac{\partial \mathcal{J}}{\partial \alpha} - \frac{1}{\mathcal{J}} \frac{\partial}{\partial \theta} \left(\frac{B_x}{B^2} \right) + 2\kappa_g. \end{cases} \quad (A2)$$

This can be simplified by expressing the pressure balance and the expressions for the curvature components described in Subsection II A, explicitly in the (α, ψ, θ) coordinate system, making use of the Clebsch representation for the magnetic field, $\mathbf{B} = \nabla \alpha \times \nabla \psi$. First, the pressure balance becomes

$$\mu_0 p' \nabla \psi = \frac{1}{\mathcal{J}} \left(\frac{\partial B_x}{\partial \theta} - \frac{\partial B_\theta}{\partial \alpha} \right) \nabla \alpha + \frac{1}{\mathcal{J}} \left(\frac{\partial B_\psi}{\partial \theta} - \frac{\partial B_\theta}{\partial \psi} \right) \nabla \psi, \quad (A3)$$

implying that, since the current lies in the magnetic flux surfaces

$$\frac{\partial B_x}{\partial \theta} = \frac{\partial B_\theta}{\partial \alpha} \quad \text{and that} \quad \mu_0 p' = \frac{1}{\mathcal{J}} \left(\frac{\partial B_\psi}{\partial \theta} - \frac{\partial B_\theta}{\partial \psi} \right). \quad (\text{A4})$$

Introducing this, and the fact that $B_\theta = B^2 \mathcal{J}$, in the expression for the normal and geodesic curvature

$$\begin{cases} \kappa_n = \frac{1}{B_\theta} \frac{\partial B_\psi}{\partial \theta} + \frac{1}{B_\theta} \left(\frac{g^{\alpha\psi}}{g^{\psi\psi}} \frac{\partial}{\partial \alpha} - \frac{\partial}{\partial \psi} + \frac{g^{\theta\psi}}{g^{\psi\psi}} \frac{\partial}{\partial \theta} \right) \left(\frac{B_\theta}{2} \right) - \frac{1}{\mathcal{J}} \left(\frac{g^{i\psi}}{g^{\psi\psi}} \frac{\partial}{\partial u^i} \right) \left(\frac{\mathcal{J}}{2} \right) \\ \kappa_g = \frac{\mathcal{J}}{B_\theta^2} \left(B_\theta \frac{\partial}{\partial \alpha} - B_x \frac{\partial}{\partial \theta} \right) \left(\frac{B_\theta}{2\mathcal{J}} \right). \end{cases} \quad (\text{A5})$$

Therefore, the operator Q_m^0 becomes

$$\begin{aligned} Q_m^0 &= \frac{nq - m}{n} \frac{1}{B_\theta} \left(B_x \frac{\partial}{\partial \theta} - B_\theta \frac{\partial}{\partial \alpha} \right) \Theta^\theta + \frac{\partial \Theta^\theta}{\partial \theta} + \frac{B_x}{B_\theta} \left(\frac{\partial \Theta^\alpha}{\partial \theta} + q' \right) + \frac{2}{B_\theta} \frac{\partial B_\psi}{\partial \theta} \\ &\quad + \frac{1}{B_\theta} \left(\Theta^\alpha \frac{\partial}{\partial \alpha} - \frac{\partial}{\partial \psi} + \Theta^\theta \frac{\partial}{\partial \theta} \right) B_\theta + \left(-\Theta^\zeta + \Theta^\theta \frac{m}{n} \right) Q_m^1 \\ &= \frac{nq - m}{n} \frac{\mathcal{J}}{B_\theta} \mathbf{B} \cdot \nabla \psi \times \nabla \Theta^\theta + q' \frac{B_x}{B_\theta} + \frac{1}{B_\theta} \left(\frac{\partial B_\psi}{\partial \theta} - \frac{\partial B_\theta}{\partial \psi} \right) + \left(-\Theta^\zeta + \Theta^\theta \frac{m}{n} \right) Q_m^1 \\ &= \frac{B_x q' + \mathcal{J} \mu_0 p'}{B_\theta} + \left(-\Theta^\zeta + \Theta^\theta \frac{m}{n} \right) Q_m^1 + \frac{nq - m}{n} \frac{\mathcal{J} \mathbf{B} \cdot \nabla \psi \times \nabla \Theta^\theta}{B_\theta}, \end{aligned} \quad (\text{A6})$$

with $\Theta^\zeta = \Theta^\alpha + q'\theta + q\Theta^\theta$. Using the same technique, the operator Q_m^1 simplifies to

$$Q_m^1 = -i(nq - m) \frac{B_x}{B_\theta}. \quad (\text{A7})$$

The axisymmetric limit of these equations corresponds to the work done by Ref. 6 and is discussed in Subsection III B.

APPENDIX B: MINIMIZATION OF PLASMA POTENTIAL ENERGY

The series of Eq. (18) is introduced into the plasma potential energy, given by Eq. (4), making use of the expressions for the adjoint operators U_k^T and DU_k^T of Sec. IID. This is done here term by term.

1. Line bending term

The stabilizing magnetic terms were described in Subsection II A by the term $\frac{1}{\mu_0} |Q_\perp|^2$. The parallel component, also called the magnetic compression term, was minimized to zero by the condition of Eq. (25) and the two perpendicular components, also called the line bending terms, are to be calculated independently from

$$\frac{1}{\mu_0} \left(\frac{1}{|\nabla \psi|^2} \left| \frac{1}{\mathcal{J}} \frac{\partial X}{\partial \theta} \right|^2 + \frac{|\nabla \psi|^2}{B^2} \left| \frac{1}{\mathcal{J}} \frac{\partial U}{\partial \theta} - SX \right|^2 \right). \quad (\text{B1})$$

Inserting the series of Eq. (18) then results in a contribution

$$\frac{1}{\mu_0} \frac{1}{\mathcal{J}^2 |\nabla \psi|^2} \left| \sum_m i(nq - m) X_m e^{i[nx + (nq - m)\theta]} \right|^2, \quad (\text{B2})$$

from the normal component, which directly leads to

$$\frac{1}{\mu_0} \sum_{k,m} X_k^* e^{i(k-m)\theta} \left[\left\{ (nq - k)(nq - m) \frac{1}{\mathcal{J}^2 |\nabla \psi|^2} \right\} X_m \right], \quad (\text{B3})$$

and

$$\frac{1}{\mu_0} \frac{|\nabla\psi|^2}{\mathcal{J}^2 B^2} \left| \sum_m \left[DU_m^0 - \mathcal{J}S + DU_m^1 \frac{i}{n} \frac{\partial}{\partial\psi} \right] (X_m) e^{i[n\alpha + (nq-m)\theta]} \right|^2, \quad (\text{B4})$$

from the geodesic component. Extracting the different orders in the derivatives in ψ

$$\begin{aligned} & \frac{1}{\mu_0} \sum_{k,m} X_k^* e^{i(k-m)\theta} \left[\left(DU_k^{T,0} - \mathcal{J}S + DU_k^{T,1} \frac{i}{n} \frac{\partial}{\partial\psi} \right) \left(\frac{|\nabla\psi|^2}{\mathcal{J}^2 B^2} \left(DU_m^0 - \mathcal{J}S + DU_m^1 \frac{i}{n} \frac{\partial}{\partial\psi} \right) \right) (X_m) \right] \\ &= \frac{1}{\mu_0} \sum_{k,m} X_k^* e^{i(k-m)\theta} \left[\left\{ DU_k^{T,1} \frac{|\nabla\psi|^2}{\mathcal{J}^2 B^2} DU_m^1 \right\} \left(\frac{i}{n} \right)^2 \frac{\partial^2}{\partial\psi^2} + \left\{ \left(DU_k^{T,0} - \mathcal{J}S \right) \frac{|\nabla\psi|^2}{\mathcal{J}^2 B^2} DU_m^1 \right. \right. \\ & \quad \left. \left. + DU_k^{T,1} \frac{|\nabla\psi|^2}{\mathcal{J}^2 B^2} \left(DU_m^0 - \mathcal{J}S \right) + DU_k^{T,1} \frac{i}{n} \frac{\partial}{\partial\psi} \left(\frac{|\nabla\psi|^2}{\mathcal{J}^2 B^2} DU_m^1 \right) \right\} \left(\frac{i}{n} \right) \frac{\partial}{\partial\psi} \right. \\ & \quad \left. + \left\{ \left(DU_k^{T,0} - \mathcal{J}S \right) \frac{|\nabla\psi|^2}{\mathcal{J}^2 B^2} \left(DU_m^0 - \mathcal{J}S \right) + DU_k^{T,1} \frac{i}{n} \frac{\partial}{\partial\psi} \left(\frac{|\nabla\psi|^2}{\mathcal{J}^2 B^2} \left(DU_m^0 - \mathcal{J}S \right) \right) \right\} \right] (X_m), \quad (\text{B5}) \end{aligned}$$

with the surface term, discussed in Eq. (32) for the adjoint operator of U_k^* equal to

$$-\frac{1}{\mu_0} \left[\mathcal{J} \frac{i}{n} DU_k^{1*} X_k^* e^{i(k-m)\theta} \frac{|\nabla\psi|^2}{\mathcal{J}^2 B^2} \left(DU_m^0 - \mathcal{J}S + DU_m^1 \frac{i}{n} \frac{\partial}{\partial\psi} \right) (X_m) \right]_{\psi_a}^{\psi_s}. \quad (\text{B6})$$

2. Ballooning term

The term that can be driven unstable by a pressure gradient oriented in the opposite direction than the curvature is the origin of the ballooning and interchange instability and has a contribution to the plasma potential energy equal to

$$-2Xp' (X^* \kappa_n + U^* \kappa_g), \quad (\text{B7})$$

that leads to

$$\begin{aligned} & \sum_{k,m} (-2) X_k^* e^{i(k-m)\theta} \left[p' \kappa_n X_m + U_k^T (\kappa_g p' X_m) \right] \\ &= \sum_{k,m} (-2) X_k^* e^{i(k-m)\theta} \left[\left\{ \kappa_g p' U_k^{T,1} \right\} \frac{i}{n} \frac{\partial}{\partial\psi} + \left\{ p' \kappa_n + \left(U_k^{T,0} + U_k^{T,1} \frac{i}{n} \frac{\partial}{\partial\psi} \right) (\kappa_g p') \right\} \right] X_m, \quad (\text{B8}) \end{aligned}$$

and a surface term

$$\left[2\mathcal{J} \frac{i}{n} U_k^{1*} X_k^* e^{i(k-m)\theta} p' \kappa_g X_m \right]_{\psi_a}^{\psi_s}. \quad (\text{B9})$$

3. Kink term

The kink term represents the term that can be driven unstable by a parallel current. It has a contribution equal to

$$\frac{1}{\mathcal{J}} \frac{\partial}{\partial\theta} (\sigma X^*) U + S \sigma X^* X + \sigma \frac{U^*}{\mathcal{J}} \frac{\partial X}{\partial\theta}, \quad (\text{B10})$$

which leads to

$$\begin{aligned}
& \sum_{k,m} X_k^* e^{i(k-m)\theta} \left[\frac{1}{\mathcal{J}} \frac{\partial \sigma}{\partial \theta} U_m(X_m) - i(nq - k) \frac{\sigma}{\mathcal{J}} U_m(X_m) + S\sigma X_m + U_k^T \left(\frac{\sigma}{\mathcal{J}} i(nq - m) X_m \right) \right] \\
&= \sum_{k,m} X_k^* e^{i(k-m)\theta} \left[\left\{ \frac{\sigma}{\mathcal{J}} \left(U_k^{T,1} i(nq - m) - U_m^1 i(nq - k) \right) - 2p' \kappa_g U_m^1 \right\} \frac{i}{n} \frac{\partial}{\partial \psi} \right. \\
& \left. + \left\{ \frac{\sigma}{\mathcal{J}} \left(i(nq - m) U_k^{T,0} - i(nq - k) U_m^0 \right) + S\sigma - U_k^{T,1} \frac{1}{n} \frac{\partial}{\partial \psi} \left(\frac{\sigma}{\mathcal{J}} (nq - m) \right) - 2p' \kappa_g U_m^0 \right\} \right] X_m, \quad (\text{B11})
\end{aligned}$$

and surface term

$$\left[\frac{1}{n} U_k^1 X_k^* e^{i(k-m)\theta} \sigma(nq - m) X_m \right]_{\psi_a}^{\psi_s}. \quad (\text{B12})$$

4. Hermitian form

Combining the contributions from all the terms, the expression for the plasma potential energy now has the form:

$$\frac{1}{2} \sum_{k,m} \int_{\psi_a}^{\psi_s} d\psi \left[d\theta \mathcal{J} X_k^* e^{i(k-m)\theta} \left\{ PV_{k,m}^0 + PV_{k,m}^1 \left(\frac{i}{n} \right) \frac{d}{d\psi} + PV_{k,m}^2 \left(\frac{i}{n} \right)^2 \frac{d^2}{d\psi^2} \right\} \right] X_m, \quad (\text{B13})$$

where the coefficients $PV_{k,m}^i$ can be simplified to a compact and visibly Hermitian form.

The coefficient $PV_{k,m}^0$ is given by a part

$$\begin{aligned}
\widetilde{PV}_{k,m}^0 &= \frac{1}{\mu_0} \left\{ (nq - k)(nq - m) \frac{1}{\mathcal{J}^2 |\nabla\psi|^2} \right\} - 2 \left\{ p' \kappa_n + \left(U_k^{T,0} + U_k^{T,1} \frac{i}{n} \frac{\partial}{\partial \psi} \right) (\kappa_g p') \right\} \\
&+ \frac{1}{\mu_0} \left\{ \left(DU_k^{T,0} - \mathcal{J}S \right) \frac{|\nabla\psi|^2}{\mathcal{J}^2 B^2} (DU_m^0 - \mathcal{J}S) + DU_k^{T,1} \frac{i}{n} \frac{\partial}{\partial \psi} \left(\frac{|\nabla\psi|^2}{\mathcal{J}^2 B^2} (DU_m^0 - \mathcal{J}S) \right) \right\} \\
&+ \left\{ \frac{\sigma}{\mathcal{J}} \left(i(nq - m) U_k^{T,0} - i(nq - k) U_m^0 \right) + S\sigma - U_k^{T,1} \frac{1}{n} \frac{\partial}{\partial \psi} \left(\frac{\sigma}{\mathcal{J}} (nq - m) \right) - 2p' \kappa_g U_m^0 \right\} \\
&= \frac{1}{\mu_0} \frac{|\nabla\psi|^2}{\mathcal{J}^2 B^2} (DU_k^{0*} - \mathcal{J}S) (DU_m^0 - \mathcal{J}S) + \frac{1}{\mathcal{J}} \frac{\partial \sigma}{\partial \theta} (U_k^{0*} + U_m^0) + \frac{1}{\mu_0} \frac{(nq - k)(nq - m)}{\mathcal{J}^2 |\nabla\psi|^2} \\
&+ \frac{\sigma}{\mathcal{J}} \left(i(nq - m) U_k^{0*} - i(nq - k) U_m^0 \right) - 2p' \kappa_n + S\sigma, \quad (\text{B14})
\end{aligned}$$

and some more terms equal to

$$\begin{aligned}
& \frac{1}{\mathcal{J}} \frac{\partial \sigma}{\partial \theta} \frac{1}{\mathcal{J}} \frac{i}{n} \frac{\partial}{\partial \psi} (U_k^{1*} \mathcal{J}) + U_k^{1*} \frac{i}{n} \frac{\partial}{\partial \psi} \left(\frac{1}{\mathcal{J}} \frac{\partial \sigma}{\partial \theta} \right) - U_k^{1*} \frac{1}{n} \frac{\partial}{\partial \psi} \left(\frac{\sigma}{\mathcal{J}} (nq - m) \right) + \frac{DU_k^{1*}}{\mu_0} \frac{i}{n} \frac{\partial}{\partial \psi} \left(\frac{|\nabla\psi|^2}{\mathcal{J}^2 B^2} (DU_m^0 - \mathcal{J}S) \right) \\
&+ \frac{1}{\mathcal{J}} \frac{i}{n} \frac{\partial}{\partial \psi} (U_k^{1*} \mathcal{J}) \frac{\sigma}{\mathcal{J}} i(nq - m) + \frac{1}{\mathcal{J}} \frac{i}{n} \frac{\partial}{\partial \psi} (DU_k^{1*} \mathcal{J}) \left(\frac{1}{\mu_0} \frac{|\nabla\psi|^2}{\mathcal{J}^2 B^2} (DU_m^0 - \mathcal{J}S) \right) \\
&= \frac{1}{\mathcal{J}} \frac{i}{n} \frac{\partial}{\partial \psi} \left(U_k^{1*} \left(\frac{\partial \sigma}{\partial \theta} + \sigma i(nq - m) \right) + DU_k^{1*} \frac{|\nabla\psi|^2}{B^2} \left(\frac{DU_m^0}{\mathcal{J}} - S \right) \right), \quad (\text{B15})
\end{aligned}$$

which are proportional to the normal derivative of a part of the coefficient $PV_{k,m}^1$, to which the surface term $SV_{k,m}^0$ is proportional as well.

The coefficient $PV_{k,m}^1$ is given by

$$\begin{aligned}
PV_{k,m}^1 &= \frac{1}{\mu_0} \left\{ (DU_k^{T,0} - \mathcal{J}S) \frac{|\nabla\psi|^2}{\mathcal{J}^2 B^2} DU_m^1 + DU_k^{T,1} \frac{|\nabla\psi|^2}{\mathcal{J}^2 B^2} (DU_m^0 - \mathcal{J}S) + DU_k^{T,1} \frac{i}{n} \frac{\partial}{\partial\psi} \left(\frac{|\nabla\psi|^2}{\mathcal{J}^2 B^2} DU_m^1 \right) \right\} \\
&\quad - 2 \left\{ \kappa_g p' U_k^{T,1} \right\} + \left\{ \frac{\sigma}{\mathcal{J}} \left(U_k^{T,1} i (nq - m) - U_m^1 i (nq - k) \right) - 2p' \kappa_g U_m^1 \right\} \\
&= \frac{1}{\mu_0} \frac{|\nabla\psi|^2}{\mathcal{J}^2 B^2} [(DU_k^{0*} - \mathcal{J}S) DU_m^1 + (DU_m^0 - \mathcal{J}S) DU_k^{1*}] + \frac{1}{\mathcal{J}} \frac{\partial\sigma}{\partial\theta} (U_m^1 + U_k^{1*}) \\
&\quad + \frac{\sigma}{\mathcal{J}} \left(U_k^{1*} i (nq - m) - U_m^1 i (nq - k) \right) + \frac{1}{\mu_0} \frac{1}{\mathcal{J}} \frac{i}{n} \frac{\partial}{\partial\psi} \left(\frac{|\nabla\psi|^2}{\mathcal{J} B^2} DU_m^1 DU_k^{1*} \right), \tag{B16}
\end{aligned}$$

where the last term is proportional to the normal derivative of the coefficient $PV_{k,m}^2$. The other terms of $PV_{k,m}^1$ can be written as the sum of

$$\widetilde{PV}_{k,m}^1 = \frac{1}{\mu_0} \frac{|\nabla\psi|^2}{\mathcal{J}^2 B^2} (DU_k^{0*} - \mathcal{J}S) DU_m^1 + \frac{U_m^1}{\mathcal{J}} \left(\frac{\partial\sigma}{\partial\theta} - \sigma i (nq - k) \right), \tag{B17}$$

and its conjugate. Also, the surface term $PS_{k,m}^1$ is proportional to $PV_{k,m}^2$.

The coefficient $PV_{k,m}^2$ is given by

$$PV_{k,m}^2 = \widetilde{PV}_{k,m}^2 = \frac{1}{\mu_0} \frac{|\nabla\psi|^2}{\mathcal{J}^2 B^2} DU_m^1 DU_k^{1*}, \tag{B18}$$

which cannot be simplified any further.

Bringing it all together results in the terms $PV_{k,m}^i$ stated in Subsection II E.

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