Symmetry breaking of ion temperature gradient mode structure: From local to global analysis

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The 2D mode structure symmetry breaking of the ion temperature gradient mode is studied analytically and numerically based on the mixed initial-value-eigenvalue approach, the Gyrokinetic PIC code ORB5 and the gyrokinetic Eulerian code GKW. The radial propagation and amplitude variation, in terms of the real and imaginary parts of the generalized “tilting parameter” \( \theta_k \), are treated in the framework of the Mode Structure Decomposition approach. The radial symmetry breaking is shown to be intimately coupled to the parallel symmetry breaking. In particular, \( \text{Im}\{\theta_k\} \) can lead to the increase in the local growth rate and the absolute value of the real frequency, as well as to parallel symmetry breaking. The complex \( \theta_k \) can be measured in global simulations and accounted for in local simulations. This provides a way to include global effects related to the mode radial propagation and the intensity gradient in local descriptions and can be important for the study of momentum transport. [http://dx.doi.org/10.1063/1.4978947]

INTRODUCTION AND MOTIVATION

In a toroidal plasma, the symmetry breaking of the two dimensional \((r, \theta)\) mode structure is related to Reynolds stress as well as wave-particle resonances and is important for understanding the toroidal momentum transport, in particular, the off-diagonal or intrinsic momentum transport, in tokamak plasmas (here, \( r, \theta \) are coordinates in the radial and poloidal directions, respectively).¹–³ While the “tilting angle” of the 2D mode structure has been observed to coincide with intrinsic momentum transport based on large scale global simulations and local analysis,⁴ the intensity gradient mechanism has also been proposed to explain the \( \{k_i\} \) generation and the consequent parallel residual stress based on fluid equations and simplified geometry.⁵ A useful theoretical tool for the study of symmetry breaking is the ballooning formalism, where the “tilting angle” \( \theta_k \) serves as an important parameter accounting for parallel symmetry breaking.⁶ While most works treat the “tilting angle” as a real number,⁴,⁷–⁹ a complex “tilting angle” parameter \( \theta_k \) has been proposed to describe the radial propagation and radial intensity gradient with its real part \( \theta_{kr} \) and imaginary part \( \theta_{ji} \),¹⁰ so that the originally proposed profile shearing mechanism⁴ and the intensity gradient mechanism⁵ can be described on the same footing and compared in different parameter regimes. The effect of complex \( \theta_k \) was also investigated in Refs. ¹¹ and ¹² for analyzing the radial mode structures and non-local couplings of Toroidal Alfvén Eigenmodes. In this work, the mixed initial-value-eigenvalue approach is applied to the calculation of the global solution order by order and compared with global gyrokinetic simulations using ORB⁵¹³,¹⁴ and GKW¹⁵ for Cyclone parameters used in Ref. ¹⁶. The results demonstrate the importance of \( \theta_{ji} \) in the construction of the fluctuation radial envelope and of the symmetry breaking of the parallel mode structure. The radial and parallel symmetry breakings are shown to be intimately connected in the presence of magnetic shear.

Identifying the effect of \( \theta_{ji} \) is important not only for the understanding of the basic physics of mode structure symmetry breaking and intrinsic rotation but also for the improvement and proper formulation of local theory and related simulation codes.¹⁵,¹⁷ This work aims at providing

1. a theoretical tool for the study of different symmetry breaking mechanisms⁴,⁵ and various momentum transport mechanisms¹³,¹⁸,¹⁹ in the framework of the mixed initial-value-eigenvalue approach or the mixed WKB-full-wave approach;¹¹,²⁰,²¹
2. a connection between information delivered by global eigenvalue initial value codes and local limits of global codes.¹⁵,¹⁷ In particular, the mixed approach applies the eigenvalue approach and the initial value approach in the parallel and radial directions, respectively;
3. proper formulation of local simulations¹⁵,¹⁷ by introducing turbulence intensity gradient in terms of the imaginary part of \( \theta_{ji} \);¹⁰
4. together with Ref. ²⁰, a theoretical tool for analyzing mode structures, in nonlinear dynamics involving mesoscale physics, by considering the nonlinear evolution of the radial mode structure.²¹,²³,²⁴ which is useful not only for symmetry breaking study but also for other fundamental physics problems, such as size effects on turbulence.²⁵

PHYSICS MODEL AND NUMERICAL IMPLEMENTATION

Models for the mixed approach

In this work, we focus on the linear global solution for a given toroidal mode number \( n \). All variables are for single \( n \) and the subscript \( n \) is omitted. The perturbed electrostatic
potential $\delta \Phi(r, \theta, \phi, t)$ is decomposed into the radial envelope $A(r, t)$ and the parallel mode structure $\delta \hat{\phi}$ using the Mode Structure Decomposition (MSD) approach\textsuperscript{20,21,26}

$$
\delta \Phi = 2\pi e^{i n_\perp q_R} \sum_{p = -\infty}^{\infty} A_p \delta \hat{\phi}(\theta + 2\pi n) e^{-2i n \eta q_R},
$$
\( p = -\infty \) for the real part and imaginary part of $\theta_k$ describe the phase variation and amplitude gradient of $A(r)$, respectively, and the $r$ dependence in $\delta \hat{\phi}$ is not written explicitly since

$$
\partial \ln \delta \hat{\phi} / \partial r \sim 1/L_{E \parallel} \ll 1/L_A
$$

($L_{E \parallel}$: the equilibrium variation spatial scale; $1/L_A \sim \partial \ln A / \partial r$). It should be noted that $\delta \hat{\phi}(\theta)$ is the parallel mode structure in mapping space\textsuperscript{20} or “covering space.”\textsuperscript{27} The connection and difference between the MSD approach and the conventional “ballooning formalism” are discussed in Ref. 20 and references therein. In this work, using MSD, we cast the two dimensional problem in $(r, \theta)$ space as two coupled one dimensional problems, i.e., the eigenvalue problem for the parallel mode structure (local solution) and the initial value problem for the radial mode structure (global solution).

We start from the linearized gyrokinetic equation for electrostatic fluctuations, described by the scalar potential only

$$
i \frac{\bar{\nu}_i}{R q} \frac{\partial}{\partial \theta} h + (\omega - \omega_D) h = (\omega - \omega_{\perp T}) f_0(\theta) \frac{e n_0}{T_i} \delta \hat{\phi}(\theta),
$$

where $\omega_D \equiv k \cdot v_D$, $v_D$ is the magnetic drift velocity

$$\omega_{\perp T} \equiv \omega_{\perp 0} \left[ 1 + \eta_i (v_i^2 + \bar{v}_i^2 - 3/2) + 2 \eta_i U_0 |\bar{v}_i| \right],
$$

where $\bar{v}_i \equiv v_i - U_i$, $U_i$ is the equilibrium parallel velocity, $\eta_i \equiv L_{ni}/L_{\perp i}$, $L_{ni} \equiv L_n/L_U$, $L_{\perp i} \equiv -d \ln n_i / dr$, $1/L_{\perp i} \equiv -d \ln T_i / dr$, and $-\delta v_E \cdot \nabla (n_0 F_0) / n_0 = i \delta \phi k \times b \cdot \nabla (n_0 F_0) / (n_0 B) \equiv i \omega_{\perp T} e \delta \phi F_0 / T_0$, $v_\perp$, $v_i$, and $v$ are normalized with $\bar{v}_i \equiv \sqrt{2T_i/m_i}$ (the tilde in $\tilde{v}_\perp$, $\tilde{v}_i$, $\tilde{e}$, and $\bar{v}_i$ indicates unnormalized), $x \equiv k \perp \rho_i = k \perp \bar{v}_i / \Omega_i = (k \perp v_i / \Omega_i)^2 v_i^2$, $k_{\perp 0}^2 \equiv k_{\perp 0}^2 f_{\perp 0} = 1 + k_{\perp 0}^2 k_{\perp 0}^2$. The equilibrium distribution function

$$F_0 = \frac{1}{(\pi m_i^2)^{3/2}} \exp \left\{ -\bar{v}_i^2 \left( \bar{v}_i - U_0 \right)^2 \right\}.
$$

In circular concentric tokamak coordinates $(r, \theta, \phi)$, which correspond to cylinder coordinates $(R, Z, \phi)$, $\omega_D$ and $\omega_{\perp 0}$ are

$$\omega_{\perp 0} = \frac{ck_\perp T_i}{eB_L}, \quad \omega_D = 2\epsilon \omega_{\perp 0} \left( \frac{v_i^2}{2} + \bar{v}_i^2 \right),
$$

$g \equiv \cos \theta + \bar{s}(\theta - \theta_k) \sin \theta$, $f_{\perp 0} = 1 + \bar{s}^2 (\theta - \theta_k)^2$,

where the real part of $\theta_k$ corresponds to the conventional “tilting angle” of the 2D mode structure.\textsuperscript{4,17} The solution of Eq. (4) for passing particles is

$$h(v_i > 0) + h(v_i < 0) = -i \tau_c \frac{e n_0}{T_i} \times \int_{-\infty}^{\infty} d\theta \frac{q_R}{|\bar{v}_i|} \times (\omega - \omega_{\perp T}) f_0(\theta) \frac{e n_0}{T_i} \delta \hat{\phi}(\theta'),
$$

where $\tau_c \equiv T_c / T_i$, $S \equiv \sin(\theta - \theta')$. With Eq. (6) substituted into the quasi-neutrality equation

$$\delta n_i = \delta n_e = (en_0/T_i) \delta \hat{\phi},
$$

the following Fredholm integral equation is obtained

$$L \delta \hat{\phi}(\theta) \equiv (1 + \tau_c) \delta \hat{\phi}(\theta) - \int_{-\infty}^{\infty} d\theta' \int_{-\infty}^{\infty} d\theta \int_{-\infty}^{\infty} d\theta' K_0 = 0,
$$

where $K_0 = K_0(v_i, v_{\perp 0}, v_{\perp 0}, \theta, \theta') \equiv -2 \pi i v_{\perp 0} \tau_c$

$$\times \frac{q_R}{|\bar{v}_i|} (\omega - \omega_{\perp T}) f_0(\theta) \delta \hat{\phi}(\theta') \exp \left\{ i \int_{\theta'}^{\theta} d\theta'' \omega - \omega_{\perp T} q_R \right\},
$$

where $v_0 = F_0 \bar{v}_i$, and whose solution gives the local dispersion relation, i.e.,

$$D_0(r, \theta_{\perp 0}, \omega_0) = 0.
$$

Note that, generally, Eq. (10) is obtained as the solution of the eigenvalue problem defined by Eq. (8) along with the specific boundary condition (B.C.), e.g., $\delta \phi \rightarrow 0$ at $\theta \rightarrow \pm \infty$ (decaying B.C.), or outgoing wave boundary condition. In practice, using the Ritz method, we write the weak form of Eq. (8) using parabolic cylinder functions as basis functions and define $D_0$ as the determinant of the eigenvalue system matrix (more details are in the “Numerical Implementation” section).

The solution of the radial envelope is obtained by following the main idea of Refs. 20 and 21, where the radial envelope $A(r, t)$ evolves along the characteristics, i.e.,

$$\frac{\partial D_0}{\partial \omega_0} \left( \frac{i}{\omega} - \omega_0 \right) A + \frac{\partial D_0}{\partial \theta_{\perp 0}} \left( -i \frac{\partial}{\partial \theta_{\perp 0}} - \theta_{\perp 0} \right) A
$$

$$+ \frac{1}{2} \frac{\partial^2 D_0}{\partial \omega_0^2} \left[ \left( -i \frac{\partial}{\partial \omega_0} - \omega_0 \right)^2 - i \frac{\partial}{\partial \theta_{\perp 0}} \theta_{\perp 0} \right] A = 0,
$$

$$A(r, t) = \exp \left\{ i \int d\eta q R (\eta_0 + \eta_{\perp 0} + \cdots) - i \omega_0 \right\},
$$

"Liu et al."

and the solution is constructed in the whole radial domain by asymptotic matching. Then, in order to obtain the global eigen-frequency, wave packets with different values of \((\omega_0, \theta_0)\) starting from the initial position need to be tracked long enough until the global solution dominates eventually, as demonstrated in Ref. 20.

While Eq. (11) demonstrates the essence of the radial mode structure evolution, we are more interested in the eventually generated global eigenmode structure, which corresponds to the \(t \to \infty\) solution of Eq. (11). With given local dispersion relation Eq. (10) as initial condition, we aim at the global solution

\[
D_G(r, \theta_G(r), \omega_G) = 0,
\]

where \(\theta_G(r)\) is \(r\) dependent and \(\omega_G\) is the global eigen-frequency (the subscript \(G\) indicates global solution). Possible ways are the application of the finite element method\(^{22}\) or WKB approach\(^{20}\) in the radial direction. In this work, instead of solving Eq. (11) directly, we specify the initial \(\theta_i(r)\) profile, e.g., \(\theta_i(r) = 0\), and calculate the local \(\omega(r)\) at various radii. Then, starting from \((\theta_i(r), \omega_i(r))\), according to the relation

\[
\Delta \omega = \frac{\partial \omega}{\partial \theta} \Delta \theta,
\]

by modifying \(\theta_i(r)\), we can approach \(\omega_G\) with a sequence of steps \(\Delta \theta\) determined by a specific scheme.

Equation (8) is formally the same as that in Ref. 28 and 29. The difference in this work includes, but is not limited to, first, the construction of a global solution based on the mixed initial-value-eigenvalue approach\(^{20}\) and the comparison with the global gyrokinetic simulation using ORB5 and GKW; second, the analysis of the symmetry breaking term, e.g., the real part of the global solution corresponds to the actually generated global eigenmode structure, which corresponds to the \(t \to \infty\) solution of Eq. (10). With given local dispersion relation Eq. (10) as initial condition, we aim at the global solution

\[
K_{qr} = -2\pi r_c \frac{v_{\perp}}{v_{\parallel}} (\Omega - \Omega_T) F_0 \times \sqrt{\frac{\pi}{\sigma_{\text{eff}}}} \left\{ \exp \left[\frac{i K_0 - K^2}{\sigma_{\text{eff}}} \right] \right\} \times \left\{ 1 + \text{erf} \left[ \sqrt{2\sigma} \left( \theta + i K_0 \right) \right] \right\} + \exp \left[ -i K_0 - K^2 \sigma_{\text{eff}} \right] \left\{ 1 + \text{erf} \left[ \sqrt{2\sigma} \left( \theta - i K_0 \right) \right] \right\},
\]

where \(\Omega \equiv \omega_0/\omega_N, \Omega_T \equiv \omega_T/\omega_N, \Omega_D \equiv \omega_D(\theta = 0)/\omega_N, \omega_N \equiv v_{\parallel}/qR\), and \(\text{erf}\) and \(\text{erfc}\) are error function and complementary error function with complex argument.

While present Eq. (14) is useful for the analysis, we extend the basis function \(\exp \left\{ -\sigma (\theta - \theta_0)^2 /2 \right\}\) to the whole set of parabolic cylinder functions in the following numerical calculation.

### Symmetry breaking in terms of \(\langle k_r \rangle, \langle \theta \rangle, \text{ and } \langle k_i \rangle\)

In mapping space (covering space), variables which describe the symmetry breaking of the parallel mode structure \(\delta \hat{\phi}\) are defined as

\[
\langle \theta \rangle \equiv \int_{-\infty}^{\infty} d\theta |\delta \hat{\phi}|^2 / I_{R0},
\]

\[
\langle k_r \rangle \equiv \frac{1}{i q R_0} \int_{-\infty}^{\infty} d\theta |\delta \hat{\phi}^* (\partial \delta \hat{\phi} / \partial \theta)| / I_{R0},
\]

with \(I_{R0} \equiv \int_{-\infty}^{\infty} d\theta |\delta \hat{\phi}|^2\). The connection among \(\langle \theta \rangle, \langle k_r \rangle\), and \(\delta \hat{\phi}\) can be demonstrated using the Weber equation. For the bounded state, the eigen function of the ion temperature gradient (ITG) mode can be approximated using the zero order parabolic cylinder function (complex Gaussian function)

\[
\text{exp} \left\{ -\sigma (\theta - \theta_0)^2 /2 \right\},
\]

where subscript \(W\) indicates “Weber” and \(\sigma\) and \(\theta_0\) are complex numbers, i.e., \(\sigma = \sigma_R + i \sigma_I, \theta_0 = \theta_0R + i \theta_0I\). Note that \(\theta_0\) is not necessarily equal to \(\theta_k\). The physically intuitive form of Eq. (18) is

\[
\delta \hat{\phi}_W = \text{exp} \left\{ -\sigma_R/2 (\theta - \theta_0)^2 - \frac{i \sigma_I}{2} (\theta - \theta_0)^2 + \frac{i \sigma^* |\sigma|^2}{2 \sigma_R \sigma_I} \phi_{\text{ITG}} \right\},
\]

\[
\theta_A = \theta_0R - \frac{\sigma_I}{\sigma_R} \theta_0I, \quad \theta_B = \theta_0R + \frac{\sigma_R}{\sigma_I} \theta_0I.
\]

Substituting Eq. (19) into Eqs. (15) and (16) yields

\[
\langle \theta \rangle_W = \theta_A - \theta_0R - \frac{\sigma_I}{\sigma_R} \theta_0I, \quad \langle k_r \rangle_W = \frac{1}{q R_0} \sigma_I (\theta_B - \theta_A) = \frac{1}{q R_0} \sigma_R |\sigma|^2 \theta_0I.
\]
Equations (20) and (21) demonstrate that \( \langle \theta \rangle \) and \( \langle k \rangle \) can be affected by both \( \theta_0 \) and \( \theta_q \). While the above analysis based on the complex Gaussian triaxial function illuminates aspects of symmetry breaking, more general asymmetric features can be obtained by considering the general form of \( \delta \phi \) and the Global-Local Connection (GLC) formula, introduced below in Definition 2.

In addition to the quantities in mapping space introduced in Eqs. (15) and (16), the corresponding physics variables in real space are defined by

\[
\langle G_{\text{phy}}(r) \rangle = \sum_{p_1, p_2} \int_{-\pi}^{\pi} d\theta d\phi \langle G(r, \theta, \phi) \rangle^2 \int_{-\pi}^{\pi} d\theta d\phi \langle \delta \phi(r, \theta, \phi) \rangle^2,
\]

where \( G \) is the variable or operator of interest, i.e., \( \theta, \partial / \partial \theta \), etc. By means of Eq. (1), the physics quantities can be represented using the Mapping-space-Real-space Connection (MRC) Formula as follows.

**Definition 1.** Mapping-space-Real-space Connection (MRC) Formula

\[
\langle G_{\text{phy}} \rangle = \sum_{p_1, p_2} \int_{-\pi}^{\pi} d\theta d\phi \langle G(r, \theta, \phi) \rangle^2 \int_{-\pi}^{\pi} d\theta d\phi \langle \delta \phi(r, \theta, \phi) \rangle^2
\]

with \( I_{R0, \text{phy}} = \sum_{p_1, p_2} \int_{-\pi}^{\pi} d\theta d\phi \langle G(r, \theta, \phi) \rangle^2 \int_{-\pi}^{\pi} d\theta d\phi \langle \delta \phi(r, \theta, \phi) \rangle^2 \).

Specific cases include, but are not limited to,

\[
\langle \theta_{\text{phy}} \rangle = \sum_{p_1, p_2} \int_{-\pi}^{\pi} d\theta d\phi \langle \theta + 2p_1 \pi \rangle \delta \phi(\theta + 2p_2 \pi) \times e^{2\pi i n (p_1-p_2) q} / I_{R0, \text{phy}},
\]

\[
\langle k_{\text{phy}} \rangle = \sum_{p_1, p_2} \int_{-\pi}^{\pi} d\theta d\phi \langle \theta + 2p_1 \pi \rangle \frac{\partial}{\partial \phi} \delta \phi(\theta + 2p_2 \pi) \times e^{2\pi i n (p_1-p_2) q} / (i q R_0 I_{R0, \text{phy}}).
\]

Note that rigorously, the integral in Eq. (23) should be replaced with a flux surface average. However, in this work we ignore the variation of the Jacobian for the sake of simplicity. For strongly ballooned parallel mode structure, \( \delta \phi \) is localized in \( \theta \in (-\pi, \pi) \) and thus only \( p_1 = p_2 = 0 \) contribution is important, i.e.,

\[
\langle G_{\text{phy}} \rangle \approx \langle G \rangle, \quad \langle \theta_{\text{phy}} \rangle \approx \langle \theta \rangle, \quad \langle k_{\text{phy}} \rangle \approx \langle k \rangle.
\]

For the weakly ballooned parallel mode structure, keeping \( p_1 = p_2 = 0 \), \( p_1 = p_2 = -1 \), \( p_1 = p_2 = 1 \), \( p_1 = 0, p_2 = \pm 1 \) and \( p_1 = \pm 1, p_2 = 0 \) is usually sufficient; e.g., for a purely real variable \( G_{R0} \),

\[
\langle (G_{R, \text{phy}}) I_{R0, \text{phy}} = \int_{-\pi}^{\pi} d\theta d\phi \langle \delta \phi \rangle^2 + 2Re \left\{ \int_{-\pi}^{\pi} d\theta d\phi \langle \delta \phi \rangle^{\ast} (\theta - 2\pi) \delta \phi \right\}.
\]

The small magnitude radial oscillation with

\[
\hat{k}_{\alpha} \approx 2\pi n q, \quad \hat{\lambda}_{\alpha} \approx 1/(n q),
\]

can be readily predicted by noticing the factor \( \exp \{2\pi i n q\} \), as shown in Fig. 4. In addition, a smaller scale oscillation with \( \hat{\lambda}_{\alpha} \approx 2/(n q) \) can also be predicted due to contribution from \( p_1 = 1, p_2 = -1 \), \( p_1 = -1, p_2 = 1 \), etc., which has even smaller magnitude and is not considered in this work.

In general, the radial and parallel mode structures are intimately coupled and, thus, the same applies to symmetry breaking. An identity can be obtained in mapping space as follows.

**Definition 2.** Parallel-Radial Connection (PRC) formula, which can also be viewed as Global-Local Connection (GLC) formula. By definition

\[
i (k_{\alpha}) = \int_{-\infty}^{\infty} d\theta d\phi \langle -\text{in} q \theta + \text{in} q \theta \rangle \delta \phi / I_{R0},
\]

we have the PRC formula (from the viewpoint of underlying physics); or the GLC formula (from the viewpoint of global-oriented simulation introduced later)

\[
\theta_k = \frac{k_{\alpha}}{\text{in} q} + \langle \theta \rangle,
\]

where \( \theta_k \) is defined in Eq. (2), whose real part is the traditional “tilting angle,” \( \langle \theta \rangle \) is defined in Eq. (15) and approximated with Eq. (25), and \( k_{\alpha} \) can be connected to the average radial derivative of \( \phi \) in global simulation

\[
\langle k_{\alpha} \rangle \approx \langle k_{\text{phy}} \rangle,
\]

where \( \langle \ldots \rangle \) is defined in Eq. (22). Note that the GLC formula is a natural result of the MSD approach and related previous works 11, 20 and is explicitly written here only for the potential benefit to simulation diagnosis and proper formulation of local simulations. As already discussed for Eq. (27), in strongly ballooning limit, Eq. (32) is more applicable while for the weakly ballooning case, small amplitude radial oscillations characterized by Eq. (29) are expected.

The GLC formula can be used for different purposes as follows:

1. Verification of the scale separation in the MSD 20 and in local simulations 15, 17. The approximation in Eq. (32) originates from Eq. (3) as well as from the difference between mode structure representations in mapping space and real space, as shown in the MRC formula. By comparing
$\theta_k$ obtained from the Wave Packet Calculation (WPC) and $(\langle k_x \phi_h \rangle)/nq' + (\langle \theta \phi_h \rangle)$ obtained from the global simulation, the applicability of Eq. (3) used in WPC can be checked.

2. Choice of the parameter $\theta_k$ to be used in local simulations consistently with global simulations or global theory. In Eq. (31), the left hand side is the input of local simulations and the right hand side variables can be obtained from global simulations. In particular, the real and imaginary parts can be separately considered depending on the case of interest

$$\theta_{kr} = \frac{Re\{\langle k_r \rangle\}}{nq'} + \langle \theta \rangle, \quad (33)$$

$$\theta_{ri} = \frac{Im\{\langle k_r \rangle\}}{nq'}. \quad (34)$$

If only the real part of $\theta_k$ is of interest, as done by previous works, only Eq. (33) is needed.

**Numerical implementation**

**Normalization.** Adopting the following normalizations for velocities and frequencies:

$$v_N = v_n, \quad \omega_N = \omega_n = \frac{v_n}{qR} \quad (35)$$

Eq. (9) yields

$$K_0 = -2\pi v_\perp \Omega - \Omega_T \frac{x(x')}{|v||} J(x)J(x') F_0 \phi'(\theta')$$

$$\times \exp \left[ i \int_0^{\theta} d\theta' \frac{\Omega - \Omega_T}{|v||} \right], \quad (36)$$

$$\Omega_T = (1 + \eta)\Omega_i, \quad \Omega_i = -\frac{k_0 \rho_s q}{\epsilon_n},$$

$$\Omega_D = k_0 \rho_s q \left( \frac{v_n^2}{2} + \frac{v_r^2}{2} \right),$$

where $\epsilon_n = L_n/R$.

**Ritz method for solving the quasi-neutrality equation.** The solution $\hat{\phi}$ is approximated using parabolic cylinder functions

$$\hat{\phi} = \sum l \hat{\phi}_l \phi_l (\theta - \theta_c), \quad (38)$$

$$h_l (\theta) = \exp \left[ - (c_1 \theta)^2 / 2 \right] \sqrt{c_1 / 2! \sqrt{\pi}}$$

where $c_1$ and $\theta_c$ are adjustable complex variables

$$\int_{-\infty}^{\infty} dx h_l(x) h_m(x) = \delta_{lm} \quad (39)$$

and $H_l$ is the $l$'th Hermite polynomial, i.e.,

$$H_0(x) = 1, \quad H_1(x) = 2x, \quad H_2(x) = 4x^2 - 2, \quad H_3(x) = 8x^3 - 12x, \ldots$$

Equation (8) is solved as an eigenvalue problem

$$M_{ml} \delta \phi_l = 0, \quad (40)$$

$$M_{ml} = (1 + \tau) \delta_{ml} - \int_0^{\infty} d\theta h_m (\theta) \int_0^{\infty} dv \left[ \int_0^{\infty} d\theta' K_{0,l}, \quad (41)$$

where $K_{0,l}$ has the same form as $K_0$ in 9 except that $\hat{\phi}$ is replaced with $\hat{\phi}_l (\theta)$, and the parallel mode structure is constructed according to Eq. (38). While the Ritz method is similar to that used in the FULL code, our method is extended to complex space and thus the argument can be complex. A practical benefit is to choose a complex $c_1$ and $\theta_c$ to achieve more efficient convergence with a smaller number of basis functions.

**Radial solution.** In order that the initially specified $[\theta_{kr}(r), \omega_r(\theta_k), \omega_G]$ converges to $[\theta_{kr}(r), \omega_G]$ as indicated in Eq. (13), we choose

$$\Delta \theta_k = \Delta \tau \frac{\partial \omega}{\partial r}, \quad (42)$$

where $\Delta \tau$ is an adjustable complex small parameter. The radial derivative is estimated with spline interpolation with the zero second derivative at inner and outer boundaries. In addition, a smoothing procedure is applied to $\theta_k$ using a global polynomial fitting or a local regression based on weighted linear least squares and a first or second degree polynomial model. When the global solution $\omega(r) = \omega_G$ is approached, $\Delta \theta_k \rightarrow 0$ and the convergent solution is obtained. In practice, by choosing $\Delta \tau = 0.01 \sim 0.02$ and $\Delta \tau = 0$, we obtain the convergent solution in several hundreds of iterations.

The choice of $\Delta \tau$ corresponds to the initial value approach and $\Delta \tau$ corresponds to $\Delta \tau$. Starting from a given time $t_0$, $\partial \omega / \partial r$ leads to the increment of the radial phase derivative $\Delta \tau (\partial \omega (r,t) / \partial r)$ from $t_0$ to $t_1$, i.e., $nq \theta_k (t = t_1) = nq \theta_k (t = t_0) + \Delta \tau (\partial \omega (r,t) / \partial r)$, where $\Delta \tau = t_1 - t_0$.

Thus, the time evolution of $\theta_k$ is given by

$$\frac{d \theta_k}{dt} = \sigma_i \frac{\partial \omega}{\partial r}, \quad (43)$$

where $\sigma_i$’s value is chosen according to $\omega_G$’s approximated value, numerical convergence requirements, and other considerations. With an appropriate $\sigma_i$, Eq. (43) converges to

$$\frac{d \theta_{kr}(r)}{dt} = \sigma_i \frac{\partial \omega_G}{\partial r} = 0. \quad (44)$$

While Eq. (44) is simple and physically intuitive, it is not the most efficient way. More discussion on the numerical implementation is beyond the scope of this paper and will be reported in a dedicated work in the future.
is ignored in Eq. ITG mode with adiabatic electrons obtained by WPC frequency. The safety factor profile is Cyclone case parameters are used, with circular concentric magnetic equilibrium. The safety factor profile is noted that the local equilibrium values enter Eq. (40) in terms of \( r, T_i, q, \xi, \epsilon_a, \eta_i \) while the higher order term in \( B \) is ignored in Eq. (40), i.e., \( B(r, \theta) \approx B_0 \) in \( \rho_i \).

### NUMERICAL RESULTS AND DISCUSSIONS

#### Parameters

The parameters are the same as those in Ref. 16. Cyclone case parameters are used, with circular concentric magnetic equilibrium. The safety factor profile is

\[
q(r) = 2.52\bar{r}^2 - 0.16\bar{r} + 0.86,
\]

(45)

where \( \bar{r} \equiv r/a \). The temperature and density profiles and the corresponding normalized logarithmic gradients are given by

\[
\frac{A(r)}{A(r_0)} = \exp \left\{-\kappa_A W_A \frac{a}{L_\text{ref}} \tanh \left(\frac{r - r_c}{W_A a}\right)\right\},
\]

(46)

\[
\frac{L_\text{ref}}{L_A} = -\frac{d}{dr} \ln A = \kappa_A \cosh^{-2} \left(\frac{r - r_c}{W_A a}\right),
\]

(47)

where the subscript “\( c \)” denotes the center of the gradient and the values of \( r_c, W_A, \) etc., are in Table I. It should be noted that the local equilibrium values enter Eq. (40) in terms of \( r, T_i, q, \xi, \epsilon_a, \eta_i \) while the higher order term in \( B \) is ignored in Eq. (40), i.e., \( B(r, \theta) \approx B_0 \) in \( \rho_i \).

#### Numerical results

**Verification and validation: Growth rate and real frequency.** The growth rate and the real frequency of the ITG mode with adiabatic electrons obtained by WPC local calculations with \( \theta_h = 0 \) are compared with the HD7 results in Ref. 29 and ORB5 global simulations, as shown in Fig. 1, where WPC and WPC-QT are defined as follows.

**Definition 3.** The WPC result refers to the solution of the ITG equations with the following approximations: only the solution for passing ions is kept; well circulating particles (constant \( v_{||} \) along trajectories); \( B \approx B_0 \) (magnitude); \( J_0(\chi) \approx \exp \{-\chi^2/4\} \). The former three are also adopted in Ref. 29.

**Definition 4.** The WPC Quasi-toroidal (WPC-QT) result refers to the solution of the ITG equations with \( g = 1 \) in \( \omega_D \) in addition to Definition 3.

The numerical verification of WPC is demonstrated in the left frame of Fig. 1, where parameters in Fig. 3 of Ref. 29 are adopted. The WPC results agree with the HD7 results in Ref. 29. The small discrepancy can be due to the approximation \( J_0(\chi) \approx \exp \{-\chi^2/4\} \) used in WPC.

The validation of the simplified model used in WPC is demonstrated in the right frame of Fig. 1. It illustrates that the frequently used model Eqs. (8) and (9)\(^\text{28,29}\) capture the main trend of the ITG mode growth rate and frequency versus \( n \) compared to the gyrokinetic simulation (ORB5), although a discrepancy exists. The enhanced \( \omega_D \) adopted in the quasi-toroidal model (WPC-QT) leads to an increase in the growth rate as compared with the more realistic \( \omega_D \) model (WPC). The ORB5 results are from global simulations, while the WPC and HD7 results are from local simulations. Considering that, generally, the local growth rate must be larger than that of the global mode structure, the reduced gyrokinetic equation used in WPC (without QT approximation) underestimates the growth rate. The discrepancy can be due to the approximation in Definition 3. In this work, we will focus on the mixed initial-value-eigenvalue approach with this acceptable discrepancy.

**Construction of global solution using mixed approach.** The typical 2D ITG mode structure is shown in Fig. 2 (left frame). By mode structure “symmetry breaking,” we refer to

1. the radial symmetry breaking, i.e., the radial propagation and amplitude variation in terms of \( \theta_h \) and \( \theta_l \) respectively;
2. the parallel symmetry breaking, i.e., the average poloidal location \( \langle \langle \theta_{hph} \rangle \rangle \rangle \) and average parallel wave vector \( \langle \langle k_{||,p} \rangle \rangle \rangle \) of the parallel mode structure.

The radial symmetry breaking and parallel symmetry breaking are coupled together, constraint by the eigenmode equation. From Fig. 2 (left), the radial symmetry breaking can be inferred from the radial propagation along \( \theta = 0 \). While the \( \theta_{LR} \) effect has been studied in previous

### Table I. Parameters for ITG with adiabatic electrons, where \( \rho_i = c_i/\Omega_i, \) \( c_i = \sqrt{T_i/m_i} \) (same as those in Ref. 16).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( r_c/a )</td>
<td>0.5</td>
</tr>
<tr>
<td>( a/\rho_0 )</td>
<td>0.36</td>
</tr>
<tr>
<td>( T_i/T_e )</td>
<td>180</td>
</tr>
<tr>
<td>( R_0/L_\text{ref} )</td>
<td>1</td>
</tr>
<tr>
<td>( \kappa_A )</td>
<td>1</td>
</tr>
<tr>
<td>( W_A = W_T )</td>
<td>6.69</td>
</tr>
<tr>
<td>( \kappa_s )</td>
<td>2.23</td>
</tr>
<tr>
<td>( \epsilon_a )</td>
<td>0.3</td>
</tr>
</tbody>
</table>

**FIG. 1.** Left: numerical verification of WPC (crosses) compared with HD7 (dashed/solid lines are with/without quasi toroidal approximation, respectively). Parameters in Ref. 29 are adopted, i.e., \( \epsilon_a = 1 \), \( q = 2.0 \), \( \delta = 1.0 \), \( \epsilon_s = 0.2 \), \( \eta_i = 1.5 \), 2, 3. Right: formulation validation for WPC and HD7 compared with ORB5, where Cyclone parameters are used as shown in Table I.
publications,\textsuperscript{4,15} in this work the effects of $\theta_{Iq}$ are also studied. As shown in Fig. 2 (right), $\theta_{Iq}$ can reach $\sim 0.5$ at radii of our interest $r \in (0.3, 0.6)$. It is also noted that since $(1/|nq_0|)^2 \partial(nq_0 \theta_{Iq})/\partial r$ is relatively small compared with $\theta_{Iq}^2$ for the present parameters, in the following analysis, this focusing/de-focusing term\textsuperscript{20,21} is neglected.

The global solution is obtained by solving Eqs. (40) and (43) as shown in Fig. 3. The growth rate and frequency at different radii (left frame) illustrate the local eigenvalue $\omega$ with $\theta_{Iq} = 0$ (black dashed line) as initial guess solution, and the convergent global solution (blue dotted line). The global solution $\theta_{Iq}(r)$ constructed using WPC (blue dotted line) agrees with that from ORB5 and GKW global simulations (black line and red dotted line on the right). It should be noted that in GKW, $\theta_{Iq}$ is directly calculated in Clebsch coordinates while in ORB5, $\theta_{Iq}$ is calculated from $\langle |k_r| \rangle$ and $\langle \theta_{r,phy} \rangle$ in $(r, \theta, \phi)$ coordinates and by using Eq. (31). The agreement between the ORB5 and GKW results demonstrates the validity of Eq. (31). Besides $\theta_{Iq}$, the radial envelope is constructed according to Eq. (2) and shown in Fig. 2 (red dashed line), with reasonable agreement with the ORB5 result.

The symmetry breaking of the parallel mode structure in terms of $\langle \theta \rangle$ and $\langle |k_i| \rangle$ is shown in Fig. 4, with reasonable agreement among WPC, ORB5, and GKW. For $\langle \theta \rangle$, the curve crosses $\langle \theta \rangle = 0$ near the maximum amplitude location while for $\langle |k_i| \rangle$, its value does not cross zero and has the magnitude of $\sim 0.1$. Another feature as shown by the black line (WPC-MRC) is the small magnitude radial oscillation of $\langle \theta \rangle$ with radial wavelength $\lambda \approx 0.02a$, whose value agrees with that $\lambda \approx 1/(|nq|)$ predicted by Eq. (29). The magnitude

![FIG. 3. Left: the local growth rate and real frequency at different radii with $\theta_{Iq} = 0$ (black) and the global solution with converged $\theta_{Iq}$ profile (blue) for $n = 20$. Right: profiles of $h_kI$ (upper) and $h_kR$ (lower) and the comparison with those from GKW and ORB5, where GLC refers to Global-Local Connection formula in Eq. (31).](image3)

![FIG. 4. Comparison of $\langle \theta \rangle$ and $\langle |k_i| \rangle$ from WPC, ORB5, and GKW. “WPC-MRC” indicates the solution using MRC formula Eq. (23) (only $p = 0, \pm 1$ kept).](image4)
of the oscillation also has similar values among the ORB5, GKW, and WPC-MRC results, in particular, for \( \langle \theta \rangle \), which supports the validity of the theoretical analysis in Eq. (28).

The role of the complex \( \theta_k \) in global solution generation and mode structure symmetry breaking. The generation of the global mode is connected to the global correction term \( \theta_k \) in the local solution. The effects of the real and imaginary parts of \( \theta_k \) on the local eigenvalue and the parallel mode structure are shown in Figs. 5 and 6. In Fig. 5, the variation of the complex eigenvalue \( \Omega \) along \( \theta_{kr} \) and \( \theta_{il} \) corresponds to two aspects of underlying physics intuitively.

1. Along the \( \theta_{kr} \) axis (\( \theta_{il} = 0 \)), \( |Re\{\Omega\}| \) and \( Im\{\Omega\} \) decrease as \( \theta_{kr} \) increases. This behavior is connected to the phase mismatch stabilization between neighboring magnetic surfaces and the consequent growth rate/frequency suppression. The usual local studies are along this direction.\(^{4,15,31}\)

2. Along the \( \theta_{il} \) axis (\( \theta_{kr} = 0 \)), \( |Re\{\Omega\}| \) and \( Im\{\Omega\} \) increase as \( \theta_{il} \) increases. Intuitively, this behavior is connected with the global solution approaching more closely the local solution and, thus, the maximum achievable growth rate.

The global solution \( \langle \omega_G, \theta_G(r) \rangle \) shown in Fig. 3 can be interpreted as a superposition of local solutions with proper complex phases. In particular, \( \theta_{kr} \) contributes to decreasing the local growth rate near the strong drive location \( r/a \approx 0.45 \), while \( \theta_{il} \) contributes to suppressing the mode amplitude in the outer region with weaker drive. It should also be noted that Fig. 3 is for ITG with \( n = 20 \) \( (k_0\rho_i \approx 0.44) \) and adiabatic electrons using Cyclone parameters. More generally, the effect of \( \theta_{kr} \) and \( \theta_{il} \) is more complicated. For example, for \( k_0\rho_i > 1 \), \( \theta_{kr} \) can lead to the increase of \( \gamma \).\(^{31}\) The effect of \( \theta_{il} \) on \( \gamma \) in a broader parameter regime is also expected to be more complicated.

The parallel symmetry breaking is the natural feature of the global mode, as a counterpart of the radial symmetry breaking that should be expected in a nonuniform plasma equilibrium. The effect of \( \theta_{kr} \) and \( \theta_{il} \) on \( \langle k_{||} \rangle \) and \( \langle \theta \rangle \) at \( r/a = 0.5 \) is shown in Fig. 6. For the global solution, with \( \langle \theta_{kr}, \theta_{il} \rangle \) solved at every radial location, \( \langle k_{||} \rangle \) and \( \langle \theta \rangle \) are naturally determined. It should be noted that various parameters such as \( \hat{s} \) and \( k_0\rho_i \) can change the contour of \( \langle k_{||} \rangle \) and \( \langle \theta \rangle \) and lead to different results. One example is the slope sign reversal of the \( \langle k_{||} \rangle \) profile from normal \( \hat{s} \) to weak \( \hat{s} \) as shown in Refs. 10, 32, and 33 and verified by ORB5 and GKW. A simple test of the effects of \( \hat{s} \) and \( n \) is performed for a \( \langle \theta \rangle \) versus \( \theta_{il} \) scan at \( \theta_{kr} = 0 \), as shown in Fig. 7. It is shown that as \( n \) or \( \hat{s} \) increases, the \( \langle \theta \rangle \) versus \( \theta_{kr} \) is closer to \( \langle \theta \rangle = \theta_{kr} \). More generally, \( \hat{s} \), \( n \), etc, affect the contour of \( \langle \theta \rangle \) and \( \langle k_{||} \rangle \) and thus the symmetry breaking in the global mode structure.
Implications to global-oriented local simulations

We call “global–oriented local simulation” a local simulation which includes a correction to capture global effects. The global correction, expressed in terms of \( \theta_{kr} \) and \( \theta_{kl} \), is obtained either from global simulations or from a self-consistent global theory and is important for the calculation of the mode structure. Thereby, it is crucial for the study of the mode structure symmetry breaking and of momentum transport. The analysis of this work suggests how to extract a complex \( \theta_k \) from local simulations in order to replace the conventional purely real parameter \( \theta_{kr} \) in local simulations. The motivation and procedure are as follows.

The introduction of the imaginary part of \( \theta_k \), i.e., \( \theta_{kl} \), in the framework of the MSD approach, and in addition to the real part \( \theta_{kr} \) used in the conventional ballooning formalism, provides a self-consistent description of the global mode structure, which is crucial, in particular, for mode structure symmetry breaking studies. While the real part \( \theta_{kr} \), i.e., the conventional “tilting angle” along which the radial wave vector is zero, captures the phase difference between neighboring local oscillations and the corresponding decrease in the growth rate, the imaginary part \( \theta_{kl} \) accounts for the mode structure localization and the ensuing increase in the growth rate. The global mode structure is generated due to the synergistic effects of both \( \theta_{kr} \) and \( \theta_{kl} \) at each radial location; thus, it is a proper superposition of local oscillations. The symmetry breaking of the mode structure in terms of \( \langle \theta \rangle \), \( \langle k_i \rangle \), and \( \langle k_e \rangle \) is naturally recovered based on the MSD approach.

In practice, the global–oriented local simulation based on gyrokinetic codes such as GKW can be tested as follows, with \( \theta_k \) extracted from a global simulation.

1. Estimate \( \langle k_e \rangle \) and \( \langle \theta \rangle \) by using Eq. (22).
2. Calculate the complex \( \theta_k \) as the input of local simulations, according to Eq. (31), the Global-Local Connection (GLC) formula. For simulation results represented in Clebsch coordinates (GKW convention), \( \theta_k \) can be calculated directly without using Eq. (31). Note that Eq. (31) can also be used as the diagnosis for symmetry breaking in global simulations and can be easily verified. The real part, i.e., Eq. (33) demonstrates the connection between three quantities of relevance for symmetry breaking, i.e., the “tilting angle,” \( \theta_{kr} \), along which the radial wave vector is zero, the average radial wave vector \( RE(k_r) \) and the average poloidal angle \( \langle \theta \rangle \).
3. Verify that \( \langle \theta_{phy} \rangle \) and \( \langle (k_i)_{phy} \rangle \) obtained from local simulations agree with those from global simulations. More generally, verify the applicability of Eq. (27) which is used in the first step, by checking they “ballooning” character of the parallel mode structure obtained in local simulations according to Eq. (28). Usually, Eq. (27) is applicable except for very weakly ballooning structures, which require other treatments, e.g., iterations between local and global simulations, in order to choose the appropriate \( \theta_k \).

DISCUSSION AND CONCLUSION

By means of the mixed initial-value-eigenvalue approach and by comparisons with global gyrokinetic simulations using ORB5, it is demonstrated that symmetry breakings in the radial and parallel directions of the 2D mode structure are intimately connected in a toroidal plasma with magnetic shear. In the framework of the MSD approach, the radial intensity gradient is treated by introducing the imaginary part of the complex \( \theta \) parameter. This is demonstrated to be important for the construction of the global solution and for the proper treatment of symmetry breaking. The effects connected with complex \( \theta \) are also helpful to better understand the applicability of the conventional local theory and open the possibility for improved analyses that allow global effects to be included in local simulations.

The mixed approach with the complex \( \theta_k \) developed in this work provides a way to estimate the contribution of the intensity gradient and the tilting angle to the symmetry breaking and the consequent momentum transport in tokamak plasmas on the same footing. While the calculation of momentum transport is beyond the scope of this work, some qualitative discussions are as follows.

1. For linear simulation, as shown in this work, the tilting angle induced symmetry breaking \( \langle k_i \rangle \) is dominant near the strongest drive location \( r = 0.5 \) where the intensity gradient is relatively small \( \theta_{phy} \approx 0 \) near \( r = 0.5 \). In the region away from the drive center, the intensity gradient becomes stronger and thus its effect on \( \langle k_i \rangle \) generation becomes also important. As a result, the tilting angle symmetry breaking is more relevant to the generation of the parallel residual stress \( \Pi^R_{\theta\phi} \) \( \times \left( \langle k_i \rangle \delta \phi (\hat{r})^2 \right) \) near the drive center while the intensity gradient symmetry breaking becomes important away from the drive center.
2. For nonlinear simulation, the turbulence spreading during the nonlinear stage makes the intensity gradient decrease in the linear unstable region and weakens the \( \theta_{kl} \) symmetry breaking for \( \langle k_i \rangle \) generation. In the linear stable region, where the turbulence spreads in, the intensity gradient can be developed and the \( \theta_{kl} \) symmetry breaking is expected to be more important. It should be noted that for nonlinear cases, each toroidal harmonic corresponds to a \( \theta_k \), and thus, the calculation of \( \langle k_i \rangle \) and the residual stress relies on a band of toroidal harmonics. In addition, the
nonlinear source term should be considered in the radial structure equation, as demonstrated in Refs. 20 and 21, and the nonlinear effects on symmetry breaking should also be assessed.

3. In practice, the intensity gradient symmetry breaking should be assessed in particular, for the internal transport barrier (ITB) region, peripheral region (e.g., the pedestal region), and non-uniformly heated plasma (e.g., lower hybrid current drive discharge$^{22}$), where the turbulence intensity gradient is expected to be large.

Besides its relevance to the problem of momentum transport, this work can also shed light on symmetry breaking and non-perturbative features of energetic particle driven instabilities, 34,35 the interaction between impurity and micro instabilities, 36,37 global drift wave mode structures in steep gradient, 38 as well as nonlinear dynamics and meso-scale physics. 21,23

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