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To cite this article: Fulvio Zonca *et al* 2021 *J. Phys.: Conf. Ser.* **1785** 012005

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Nonlinear radial envelope evolution equations and energetic particle transport in tokamak plasmas

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Abstract. This work provides a general description of the self-consistent energetic particle phase space transport in burning plasmas, based on nonlinear gyrokinetic theory. The self consistency is ensured by the evolution equations of the Alfvénic fluctuations by means of nonlinear radial envelope evolution equations, while energetic particle fluxes in the phase space are explicitly constructed from long-lived phase space zonal structures, which are undamped by collisionless processes. As a result, this work provides a viable route to computing fluctuation induced energetic particle transport on long time scales in realistic tokamak plasmas.

1. Introduction

The role of energetic particles (EPs) in fusion plasmas is unique as they could act as mediators of cross-scale couplings [1, 2]. Energetic particle driven shear Alfvén waves (SAWs), on one hand, could provide a nonlinear feedback onto the macro-scale system via the interplay of plasma equilibrium and fusion reactivity profiles. Meanwhile, EP-driven instabilities could also excite singular radial mode structures at SAW continuum resonances, which, by mode conversion, yield microscopic fluctuations that may propagate and be absorbed elsewhere, inducing nonlocal behaviors that require a global analysis. Energetic particle transport must be described in phase space because of the underlying kinetic nature of wave-particle interactions and fluctuation excitations. The proper structures to describe such transport processes are phase space zonal structures (PSZS) [3]. Energetic particles, furthermore, may linearly and nonlinearly excite zonal field structures (ZFS), acting, thereby, as generators of nonlinear equilibria, or zonal states (ZS) that generally evolve on the same time scale of the underlying fluctuations. These issues are presented within a general theoretical framework. In particular, we present the nonlinear envelope equations (Sec. 2) that are needed to solve for the self-consistent evolution of the SAW fluctuation spectrum driven by EPs and the PSZS transport equations (Sec. 3), which determine the renormalized response of EPs including fluctuation induced transport [4]. The present approach can be extended from tokamak to more general 3D magnetic equilibria, such as stellarators, and work is in progress along these lines [5]. For the sake of conciseness and clarity, this work is limited to axisymmetric tokamaks.



2. Nonlinear envelope equations

We assume low- β tokamak plasmas with good separation of SAW and compressional Alfvén wave frequencies¹. Thus, the parallel (to the equilibrium magnetic field \mathbf{B}_0) magnetic field fluctuation, δB_{\parallel} , is obtained from the perpendicular (to \mathbf{B}_0) pressure balance [1]

$$\nabla_{\perp} (B_0 \delta B_{\parallel} + 4\pi \delta P_{\perp}) \simeq 0, \quad (1)$$

where, assuming a generally anisotropic plasma response, δP_{\perp} represents the perpendicular pressure perturbation. It is of crucial importance that δB_{\parallel} is obtained from Eq. (1) and not assumed to vanish [1]. Here and in the following, unless otherwise specified, fluctuations are intended to be “symmetry breaking”; *i.e.*, characterized by finite toroidal mode number $n \neq 0$ in the considered axisymmetric tokamak equilibrium. Having solved for δB_{\parallel} explicitly, the drift Alfvén wave (DAW) [1] fluctuation spectrum is entirely described by scalar potential, $\delta\phi$, and parallel vector potential, δA_{\parallel} . For convenience, we choose $\delta\psi$ as independent field variable instead of δA_{\parallel} , which is defined as $\nabla_{\parallel} \delta\psi \equiv -(1/c) \partial_t \delta A_{\parallel}$. In this way, vanishing of the parallel electric field for $k_{\parallel} \neq 0$ reads $\delta\phi = \delta\psi$, with \mathbf{k} the wave vector and k_{\parallel} its parallel component. Coupled nonlinear evolution equations for $\delta\phi$ and $\delta\psi$ are given by the gyrokinetic quasineutrality

$$\sum \left\langle \frac{e^2}{m} \frac{\partial \bar{F}_0}{\partial \mathcal{E}} \right\rangle_v \delta\phi + \nabla \cdot \sum \left\langle \frac{e^2}{m} \frac{2\mu}{\Omega^2} \frac{\partial \bar{F}_0}{\partial \mu} \left(\frac{J_0^2 - 1}{\lambda^2} \right) \right\rangle_v \nabla_{\perp} \delta\phi + \sum \langle e J_0(\lambda) \delta g \rangle_v = 0. \quad (2)$$

and gyrokinetic vorticity equation

$$\begin{aligned} & B_0 \left(\nabla_{\parallel} + \frac{\delta \mathbf{B}_{\perp}}{B_0} \cdot \nabla \right) \left(\frac{\delta J_{\parallel}}{B_0} \right) - \nabla \cdot \sum \left\langle \frac{e^2}{m} \frac{2\mu}{\Omega^2} \left(B_0 \frac{\partial \bar{F}_0}{\partial \mathcal{E}} + \frac{\partial \bar{F}_0}{\partial \mu} \right) \left(\frac{J_0^2 - 1}{\lambda^2} \right) \right\rangle_v \nabla_{\perp} \frac{\partial}{\partial t} \delta\phi \\ & + \sum e c \mathbf{b}_0 \times \nabla \left\langle \frac{2\mu}{\Omega^2} \bar{F}_0 \left(\frac{J_0^2 - 1}{\lambda^2} \right) \right\rangle_v \cdot \nabla \nabla_{\perp}^2 \delta\phi + \frac{c}{B_0} \mathbf{b}_0 \times \boldsymbol{\kappa} \cdot \nabla \sum \left\langle m (\mu B_0 + v_{\parallel}^2) J_0 \delta g \right\rangle_v \\ & + \delta \mathbf{B}_{\perp} \cdot \nabla \left(\frac{J_{\parallel 0}}{B_0} \right) + \sum e \left\langle J_0 \left[\frac{c}{B_0} \mathbf{b}_0 \times \nabla (J_0 \delta\phi) \cdot \nabla \delta g \right] - \frac{c}{B_0} \mathbf{b}_0 \times \nabla \delta\phi \cdot \nabla (J_0 \delta g) \right\rangle_v \\ & + \frac{c}{B_0} \mathbf{b}_0 \times \nabla \delta\phi \cdot \nabla \left[\nabla \cdot \sum \left\langle \frac{e^2}{m} \frac{2\mu}{\Omega^2} \frac{\partial \bar{F}_0}{\partial \mu} \left(\frac{1 - J_0^2}{\lambda^2} \right) \right\rangle_v \nabla_{\perp} \delta\phi \right] = 0. \end{aligned} \quad (3)$$

Equations (2) and (3) are given without derivation. Interested readers are referred to the original works for all details [1, 6, 7], including discussions of underlying assumptions, validity limits and possible further extensions. In this context, we only emphasize that Eqs. (2) and (3) contain sufficiently accurate physics descriptions derived from first principles to be applicable in most cases of practical interest, including ITER. Here, $\delta \mathbf{B}_{\perp} = (\nabla \times \mathbf{b}_0 \delta A_{\parallel})_{\perp}$, $\mathbf{b}_0 = \mathbf{B}_0/B_0$, $\boldsymbol{\kappa} = \mathbf{b}_0 \cdot \nabla \mathbf{b}_0$, $J_{\parallel 0}$ is the equilibrium parallel current density and

$$\delta J_{\parallel} \simeq -\frac{c}{4\pi} (\nabla_{\perp}^2 - \boldsymbol{\kappa} \cdot \nabla_{\perp}) \delta A_{\parallel} \quad (4)$$

is the parallel current density fluctuation. Furthermore, summation is on particle species with electric charge e , mass m , cyclotron frequency $\Omega = eB_0/(mc)$ and “renormalized” (nonlinear/evolving) equilibrium distribution function $\bar{F}_0(\mathcal{E}, \mu, P_{\phi})$, with $\mathcal{E} = v^2/2$, $\mu \simeq v_{\perp}^2/2B_0$ the leading order expression of the magnetic moment and $P_{\phi} \simeq (e/c) (F(\psi)(v_{\parallel}/\Omega) - \psi)$ the corresponding leading order toroidal canonical angular momentum, having adopted the $\mathbf{B}_0 = F(\psi) \nabla \varphi + \nabla \psi \times \nabla \theta$ representation of the tokamak equilibrium magnetic field, with (ψ, θ, φ) the toroidal flux coordinates. Thus, \bar{F}_0 as a function of invariants of motion (given with

¹ Here, using standard notation, β is the ratio of kinetic to magnetic energy density.

the desired accuracy) represents the PSZS that will be discussed below in Sec. 3. Meanwhile, J_0 is the zeroth Bessel function of argument λ , $\lambda^2 = 2\mu B_0 k_\perp^2 / \Omega^2$ and δg is the nonadiabatic particle response that satisfies the nonlinear gyrokinetic equation [8, 9] (cf. Sec. 3).

Given the strong equilibrium magnetic field, $\delta\phi$ and $\delta\psi$ are characterized by $|k_\parallel| \ll |k_\perp|$. These field aligned structures, which become nearly filamentary at high toroidal mode number n [1, 2], can be well represented as [1, 2, 10]

$$\begin{bmatrix} \delta\phi(r, \theta, \zeta) \\ \delta\psi(r, \theta, \zeta) \end{bmatrix} = 2\pi \sum_{n, \ell \in \mathbb{Z}} e^{in\zeta - inq(\psi)(\theta - 2\pi\ell)} \begin{bmatrix} \delta\hat{\phi}_n(r, \theta - 2\pi\ell) \\ \delta\hat{\psi}_n(r, \theta - 2\pi\ell) \end{bmatrix}, \quad (5)$$

where, for brevity, we have omitted time dependences, $q(\psi)$ is the safety factor, and we have introduced the field aligned toroidal flux coordinates (r, θ, ζ) that can always be constructed from (ψ, θ, φ) [11]. Equation (5) is always valid and reduces to the well known ballooning transformation [12, 13, 14] for high- n [10]. Although generally possible, using Eq. (5) does not introduce significant advantages at low- n . At moderate and/or high- n , instead, thanks to Eq. (5) representation, it is possible to treat Eqs. (2) and (3) with the formalism of wave equations in slowly evolving weakly nonuniform media [1, 2, 6, 7, 15, 16, 17] and introduce radial envelope $A_n(r, t)$, eikonal $S_n(r, t)$ and polarization vector $\hat{e}_n = [\hat{e}_{n1}(r, t), \hat{e}_{n2}(r, t)]^T$ as²

$$\begin{pmatrix} e\delta\hat{\psi}_n(r, \vartheta; t)/T_{0i} \\ e\delta\hat{\phi}_{\parallel n}(r, \vartheta; t)/T_{0i} \end{pmatrix} \equiv A_n(r, t)e^{iS_n(r, t)} \begin{pmatrix} e_1(r, t)y_1(r, \vartheta; t) \\ e_2(r, t)y_2(r, \vartheta; t) \end{pmatrix}. \quad (6)$$

Here, we have explicitly indicated time dependences, T_{0i} is the thermal ion (nonlinear) equilibrium temperature, normalizations are chosen such as $\hat{e}_n^+ \cdot \hat{e}_n = 1$, with $\hat{e}_n^+ = [\hat{e}_{n1}^*(r, t), \hat{e}_{n2}^*(r, t)]$; and $\delta\hat{\phi}_{\parallel n} \equiv \delta\hat{\phi}_n - \delta\hat{\psi}_n$ has been introduced such that $\hat{e}_n = (1, 0)^T$ and $\hat{e}_n = (0, 1)^T$ represent, respectively, pure Alfvénic and acoustic polarizations [18, 19, 20, 21]. Meanwhile, $y_{1,2}(r, \vartheta; t)$ represent parallel mode structures in the extended ballooning coordinate ϑ [6, 7], for which we assume

$$\int_{-\infty}^{\infty} |y_{1,2}(r, \vartheta; t)|^2 d\vartheta = 1. \quad (7)$$

Using this representation, and solving for the parallel mode structures, the solubility condition for Eqs. (2) and (3) can be cast as [6, 7]

$$\hat{e}_n^+ \cdot \mathbf{D}(r, t, k_{nr}, \omega_n) \cdot \mathbf{A}_n(r, t)e^{iS_n(r, t)} = \hat{e}_n^+ \cdot \mathbf{F}(r, t), \quad (8)$$

with $\mathbf{A}_n(r, t) \equiv \hat{e}_n A_n(r, t)$, $k_{nr}(r, t) = \partial_r S_n(r, t)$ and $\omega_n = -\partial_t S_n(r, t)$. Furthermore, $\mathbf{F}(r, t)$ on the right hand side symbolically denotes all nonlinear interactions and, possibly, external forcing. General expressions of $\mathbf{F}(r, t)$ can be obtained by inspection of Eqs. (2) and (3) and their lengthy form will be given elsewhere.

This structure of Eqs. (2) and (3) is particularly useful given the typical time scale ordering of DAW excitation by EPs in burning plasmas, that is $|\gamma_{Ln}| \sim \tau_{NLn}^{-1} \ll |\omega_n|$ [1], where γ_{Ln} is the growth rate of the fluctuations with toroidal mode number n and τ_{NLn} the corresponding characteristic nonlinear time scale. In fact, it is possible to argue that the time scale for the parallel mode structures to form, $\sim |\omega_n|^{-1}$, is too short for $y_{1,2}(r, \vartheta; t)$ to be modified by nonlinear interactions. Thus, $y_{1,2}(r, \vartheta; t)$ can be effectively approximated by the corresponding linear parallel mode structures, $y_{1,2}^L(r, \vartheta; t)$, which are computed once the reference (nonlinear)

² Here, $[a, b]^T$ is the standard notation of the transpose of the row vector $[a, b]$; *i.e.*, the corresponding column vector with the same components.

equilibrium is given. Adopting the standard asymptotic expansion approach, the leading order local dispersion relation

$$D_{Rn}^0(r, t, k_{nr}, \omega_n) \equiv \hat{\mathbf{e}}_n^+ \cdot \mathbf{D}_R^0 \cdot \hat{\mathbf{e}}_n = 0 \quad (9)$$

can be solved for $\omega_n = \bar{\Omega}_n(k_{nr}, r, t)$. Furthermore, $D_{Rn}^1 \equiv \hat{\mathbf{e}}_n^+ \cdot \mathbf{D}_R^1 \cdot \hat{\mathbf{e}}_n$ is the first order contribution to the real dispersion function in the asymptotic series, while $D_{An}^1 \equiv \hat{\mathbf{e}}_n^+ \cdot \mathbf{D}_A^1 \cdot \hat{\mathbf{e}}_n$ provides the leading order anti-Hermitian dispersion function, consistent with the $|\gamma_{Ln}| \sim \tau_{NLn}^{-1} \ll |\omega_n|$ ordering. Meanwhile, Eq. (8) can be solved by asymptotic perturbation expansion, which yields [1, 2, 6, 7]

$$\begin{aligned} & \frac{\partial}{\partial t} \left(\frac{\partial D_{Rn}^0}{\partial \omega_n} A_n^2 \right) - \frac{\partial}{\partial r} \left(\frac{\partial D_{Rn}^0}{\partial k_{nr}} A_n^2 \right) + 2D_{An}^1 A_n^2 - 2iD_{Rn}^1 A_n^2 \\ & + iA_n \left(\frac{\partial^2 D_{Rn}^0}{\partial k_{nr}^2} + 2 \frac{\partial \hat{\mathbf{e}}_n^+}{\partial k_{nr}} \cdot \mathbf{D}_{Rn}^0 \cdot \frac{\partial \hat{\mathbf{e}}_n}{\partial k_{nr}} \right) \frac{\partial^2 A_n}{\partial r^2} = -2ie^{-iS_n} A_n \hat{\mathbf{e}}_n^+ \cdot \mathbf{F} \\ & - \left(\hat{\mathbf{e}}_n^+ \cdot \frac{d}{dt} \hat{\mathbf{e}}_n - \frac{d}{dt} \hat{\mathbf{e}}_n^+ \cdot \hat{\mathbf{e}}_n \right) \frac{\partial D_{Rn}^0}{\partial \omega_n} A_n^2 + \left(\frac{\partial \hat{\mathbf{e}}_n^+}{\partial \omega_n} \cdot \mathbf{D}_{Rn}^0 \cdot \frac{\partial \hat{\mathbf{e}}_n}{\partial t} - \frac{\partial \hat{\mathbf{e}}_n^+}{\partial t} \cdot \mathbf{D}_{Rn}^0 \cdot \frac{\partial \hat{\mathbf{e}}_n}{\partial \omega_n} \right) A_n^2 \\ & - \left(\frac{\partial \hat{\mathbf{e}}_n^+}{\partial k_{nr}} \cdot \mathbf{D}_{Rn}^0 \cdot \frac{\partial \hat{\mathbf{e}}_n}{\partial r} - \frac{\partial \hat{\mathbf{e}}_n^+}{\partial r} \cdot \mathbf{D}_{Rn}^0 \cdot \frac{\partial \hat{\mathbf{e}}_n}{\partial k_{nr}} \right) A_n^2. \end{aligned} \quad (10)$$

The total time derivatives, where they appear, are defined as $d/dt = \partial_t + v_{gn}\partial_r$, with the group velocity $v_{gn} = -(\partial D_{Rn}^0/\partial k_{nr})/(\partial D_{Rn}^0/\partial \omega_n)$. Note that, by dropping the $\sim \partial_r^2 A_n$ term, Eq. (10) is the well-known propagation equation for wave packet amplitude and phase that can be used to derive the corresponding wave kinetic equation [15, 16, 17]. The presence of the $\sim \partial_r^2 A_n$ term makes Eq. (10) a nonlinear Schrödinger like equation (NLSE-like), which is of crucial importance for proper analysis of structure formation in strongly magnetized toroidal plasmas, where wave packets can be focused/defocused and back scattered by both nonlinearities as well as by radial nonuniformities [1, 2, 6, 7]. In fact, the peculiar NLSE-like structure of Eq. (10), different from the standard wave kinetic equation that is typically adopted in literature, is of fundamental importance not only in the description of EP induced avalanches, such as in the case of energetic particle modes (EPM) [3, 22], but also for the interaction of zonal fields and drift wave turbulence [23, 24, 25, 26, 27].

The NLSE-like Eq. (10) accounts for the effects of nonlinearities only via the nonlinear distortion of the radial envelope functions A_n 's, which are coupled together because of the explicitly nonlinear term $\sim \hat{\mathbf{e}}_n^+ \cdot \mathbf{F}$ on the right hand side. Note that the non-trivial formal effort to numerically, or – where possible – analytically, compute the elements of this equation [5] is well payed back by the reduction in dimensionality and by the fact that the various elements can be obtained by means of the linearized Eqs. (2) and (3). Even the explicit nonlinear term $\sim \hat{\mathbf{e}}_n^+ \cdot \mathbf{F}$, although formally complicated, can be calculated by averaging along the linear parallel mode structures [5]. However, we note that the nonlinear envelope functions may be completely different from those of linear eigenmodes, since nonlinearities enter on the same footing as the radial propagation of wave packets due to finite radial group velocity in the time evolving nonuniform plasma equilibrium. The generality of this approach is discussed in Refs. [1, 2, 6, 7] and goes well beyond the applicability of the wave kinetic equation, mentioned above, and of the radially local description usually adopted in flux-tube or quasilinear approaches. For this reason, this methodology is well suited to be extended to three-dimensional nonuniform plasmas, such as stellarators [14]. This approach, in particular, allows to account for flux-tubes not covering the whole flux surface in stellarator equilibria, which results in the dependence of the envelope functions on both Clebsch potentials [14]. Thus, it opens a route to systematic calculation of fluctuation induced fluxes in three-dimensional plasma equilibria. Due to the nontrivial twists that this extension of the present approach implies, it will be discussed elsewhere.

When adopted as nonlinear radial envelope evolution equation for investigating energetic particle transport due to DAW in tokamak plasmas, Eq. (10) can benefit from the theoretical framework of the general fishbone-like dispersion relation (GFLDR) [1, 6, 7], which gives

$$\begin{aligned} D_{Rn}^0(r, k_{nr}, \omega_n) + D_{Rn}^1(r, k_{nr}, \omega_n) + iD_{An}^1(r, k_{nr}, \omega_n) \\ = \delta\bar{W}_f^L(r, k_{nr}, \omega_n) + \delta\bar{W}_k^L(r, k_{nr}, \omega_n) - i\Lambda^L(r, \omega_n), \end{aligned} \quad (11)$$

and

$$e^{-iS_n} \hat{e}_n^+ \cdot \mathbf{F}/A_n = i\Lambda^{NL} - \delta\bar{W}_f^{NL} - \delta\bar{W}_k^{NL} + e^{-iS_n} \hat{e}_n^+ \cdot \mathbf{F}_{\text{ext}}/A_n. \quad (12)$$

Equations (11) and (12) account for linear (superscript L) and nonlinear (superscript NL) effects, respectively, as well as external forcing (subscript ext). Here, consistent with the GFLDR theory, Λ describes the generalized inertia due to the e.m. field behaviors on short length scales, while $\delta\bar{W}_f$ and $\delta\bar{W}_k$ account for “fluid” and “kinetic” potential energy fluctuations due to meso- and macro-scale responses [1, 2, 3, 6, 7]. From Eq. (12), in general, we can write [1]

$$\begin{aligned} e^{-iS_n} \hat{e}_n^+ \cdot (\mathbf{F} - \mathbf{F}_{\text{ext}}) = (C_{n,0} + C_{0,n}) \circ A_n(r, t) A_z(r, t) \\ + \sum_{\substack{n', n'' \neq n \\ n' + n'' = n}} C_{n', n''} \circ A_{n'}(r, t) A_{n''}(r, t) \end{aligned} \quad (13)$$

where “ $C_{n', n''}$ ” imply nonlocal interactions in the n toroidal mode number space and whose composition with (action on) $A_n(r, t)$ and/or $A_z(r, t)$ is denoted by \circ [1]. The explicit form of $C_{n', n''}$ can be deduced from the expressions of Λ , $\delta\bar{W}_f$ and $\delta\bar{W}_k$ given in Refs. [1, 2, 3, 6, 7]. Meanwhile, $A_n(r, t)$ and $A_z(r, t)$ denote, respectively, the radial envelopes of symmetry breaking fluctuations and ZFS given by $n = 0$ e.m. fields; that is, $\delta\phi_z$ and $\delta A_{\parallel z}$, noting that $\delta B_{\parallel z}$ can be explicitly solved for [28, 29] analogously to Eq. (1). The presence of finite ZFS induces, more generally, zonal structures, such as current density, temperature, etc. perturbations, which can be consistently computed from the phase space particle responses given in Sec. 3. But while $\delta\phi_z$ can be obtained from the $n = 0$ component of Eq. (2), $\delta A_{\parallel z}$ is obtained from [1]

$$\frac{\partial}{\partial t} \delta A_{\parallel z} = \left(\frac{c}{B_0} \mathbf{b}_0 \times \nabla \delta A_{\parallel} \cdot \nabla \delta \psi \right)_z. \quad (14)$$

Equation (13) accounts for three wave couplings via the $\sim C_{n', n''} \circ A_{n'}(r, t) A_{n''}(r, t)$ term, as well as for both three as well as four wave couplings (due to zero frequency ZFS) via the $(C_{n,0} + C_{0,n}) \circ A_n(r, t) A_z(r, t)$ term. This latter term also accounts for rapid distortions away from the nonlinear equilibrium that are not accounted for by the evolution of PSZS (cf. Sec. 3). In summary, Eqs. (2), (3) and (14) fully characterize the DAW fluctuation and ZFS spectrum evolution, with the NLSE-like Eq. (10) providing the nonlinear radial envelope evolution equations that account for nonlocal behaviors, structure formation, avalanches etc. [1, 2, 3]. This, of course, given PSZS, \bar{F}_0 , and nonadiabatic particle responses, δg , which are discussed in the following section.

3. Phase space zonal structures and nonlinear equilibrium

The investigation of fluctuation induced transport in burning fusion plasmas on long time scales, $\sim \mathcal{O}(k_{\perp}^3 L^3 / \lambda^3) \Omega^{-1}$, with L the macroscopic system size, poses challenging questions (cf. Ref. [30] for a recent review) especially for the description of resonant EP transport in phase space [1, 2, 3]. In fact, resonant behaviors and transport of nearly collisionless EPs generate structures in the phase space that can significantly deviate from equilibrium in the absence of fluctuations and, thus, influence transport on long time scales [4, 31]. These PSZS are characterized by

being undamped by collisionless processes and do not evolve in time in the absence of symmetry breaking fluctuations and sources/collisions [1, 3]. This property characterizes PSZS as functions of the invariants of motion in the considered reference “equilibrium”, which may be evolving in time [4]. In order to explore this more in detail, let us consider the nonlinear gyrokinetic equation in conservative form [8, 9, 30]

$$\partial_t (DF) + \partial_{\mathbf{X}} \cdot (D\dot{\mathbf{X}}F) + \partial_{\mathcal{E}} (D\delta\dot{\mathcal{E}}F) = C_g + \mathcal{S}. \quad (15)$$

where $D = B_{\parallel}^*/v_{\parallel}$ is the velocity space Jacobian, $B_{\parallel}^* = B_0 + (v_{\parallel}/\Omega)\mathbf{B}_0 \cdot \nabla \times \mathbf{b}_0$, F is the gyrocenter particle distribution function, \mathbf{X} are gyrocenter coordinates, and we have noted that \mathcal{E} and μ are constants of motion. Meanwhile, on the right hand side, C_g and \mathcal{S} denote, respectively, gyrocenter collision operator [32] and source term. When solved *ab initio*, Eq. (15) usually assumes an initial $F_0(\mathcal{E}, \mu, P_{\phi})$ that is then let evolve in time under the effect of symmetry breaking fluctuations and ZFS. Focusing on the $n = 0$ zonal particle response, F_z , and introducing the drift/banana center pull-back operator e^{-iQ_z} , with $Q_z = F(\psi)(v_{\parallel}/\Omega)k_z/(d\psi/dr)$ at leading order³, with k_z the ZFS radial wave-number,

$$F_z \equiv \bar{F}_0 + \delta F_z \equiv \bar{F}_0 + e^{-iQ_z} \delta F_{Bz}, \quad (16)$$

with δF_{Bz} the corresponding drift/banana center particle response. Note that, in this equation, δF_z is the deviation of the zonal particle response from the PSZS \bar{F}_0 that will be defined below, and that is a function of the invariants of motion but also depends explicitly on time. By definition, the initial condition on \bar{F}_0 is $\bar{F}_0(\mathcal{E}, \mu, P_{\phi}, t = 0) = F_0(\mathcal{E}, \mu, P_{\phi})$. Meanwhile, introducing the bounce averaging $\overline{(\dots)} \equiv \tau_b^{-1} \oint (\dots) d\theta/\dot{\theta}$, with $\tau_b = \oint d\theta/\dot{\theta}$ the transit/bounce time it takes to a particle to complete a poloidally closed orbit, it follows from the definitions above that

$$F_z \equiv \bar{F}_0 + e^{-iQ_z} \left(\overline{\delta F_{Bz}} \Big|_F + \delta \tilde{F}_{Bz} \right) = \bar{F}_0 + e^{-iQ_z} \left(\overline{e^{iQ_z} \delta F_z} \Big|_F + \delta \tilde{F}_{Bz} \right), \quad (17)$$

where $\delta \tilde{F}_{Bz} \equiv \delta F_{Bz} - \overline{\delta F_{Bz}}$ has zero bounce average, and the subscript F denotes the “fast” spatiotemporal micro-scales, which we intend to *ad hoc* separate from the the “slow” spatiotemporal meso- and macro-scales dependences denoted by the subscript S [4, 28, 29]. Note that, in Eq. (17), $\overline{e^{iQ_z} \delta F_z}$ is the orbit average of δF_z along the integrable particle orbit in the considered magnetic (nonlinearly evolving) “equilibrium”. Thus, Eq. (17) postulates that all the slow orbit averaged zonal particle response is included in the PSZS \bar{F}_0 , and that the residual part can only vary on “fast” spatiotemporal micro-scales or have zero orbit average. It is possible to show that the function

$$G_z = e^{-iQ_z} G_{Bz} \equiv F_z - \frac{e}{m} \langle \delta L_g \rangle_z \frac{\partial}{\partial \mathcal{E}} \Big|_{\bar{\psi}} \bar{F}_0 + \frac{F(\psi)}{B_0} \langle \delta A_{\parallel g} \rangle_z \frac{\partial}{\partial \psi} \bar{F}_0 \quad (18)$$

with angular brackets denoting gyroaveraging, $\langle \delta L_g \rangle \equiv J_0(\lambda) (\delta\phi - v_{\parallel} \delta A_{\parallel} / c) + (2m\mu/e\lambda) J_1(\lambda) \delta B_{\parallel}$, $\langle \delta A_{\parallel g} \rangle \equiv J_0(\lambda) \delta A_{\parallel}$, and $\bar{\psi} \equiv -(c/e)P_{\phi}$, satisfies the following evolution equation [28, 29]:

$$\begin{aligned} \partial_t \overline{G_{Bz}} &= -e^{iQ_z} \frac{e}{m} \partial_t \left[\langle \delta L_g \rangle_z \frac{\partial}{\partial \mathcal{E}} \Big|_{\bar{\psi}} \bar{F}_0 \right] + e^{iQ_z} \frac{F(\psi)}{B_0} \langle \delta A_{\parallel g} \rangle_z \frac{\partial}{\partial \psi} \partial_t \bar{F}_0 + \overline{e^{iQ_z} [C_g + \mathcal{S}]}_z \\ &\quad - \frac{1}{\tau_b} \frac{\partial}{\partial \psi} \left[\tau_b e^{iQ_z} \delta \dot{\psi}_z \delta F_z \right] - \frac{1}{\tau_b} \frac{\partial}{\partial \mathcal{E}} \left[\tau_b e^{iQ_z} \delta \dot{\mathcal{E}}_z \delta F_z \right] \\ &\quad - \frac{1}{\tau_b} \frac{\partial}{\partial \psi} \left[\tau_b e^{iQ_z} \delta \dot{\psi} \delta F \right]_z - \frac{1}{\tau_b} \frac{\partial}{\partial \mathcal{E}} \left[\tau_b e^{iQ_z} \delta \dot{\mathcal{E}} \delta F \right]_z, \end{aligned} \quad (19)$$

³ Note, here, that $F(\psi)$ is the expression entering the representation of \mathbf{B}_0 , not to be confused with the gyrocenter particle distribution function.

where the last two terms on the right hand side are due to symmetry breaking fluctuations only. Meanwhile, extending the definition in Eq. (18) to symmetry breaking fluctuations [1, 8, 9], and connecting the nonadiabatic particle response δg , introduced in Eqs. (2) and (3), to the perturbed gyrocenter particle distribution function, δF , we can write

$$\delta g \equiv \delta F - \frac{e}{m} \langle \delta L_g \rangle \frac{\partial}{\partial \mathcal{E}} \Big|_{\bar{\psi}} \bar{F}_0 + \frac{F(\psi)}{B_0} \langle \delta A_{\parallel g} \rangle \frac{\partial}{\partial \psi} \bar{F}_0, \quad (20)$$

which evolves in time according to the following nonlinear gyrokinetic equation

$$\begin{aligned} (\partial_t + \dot{\mathbf{X}}_0 \cdot \nabla) \delta g &= -\frac{e}{m} \partial_t \left[\langle \delta L_g \rangle \frac{\partial}{\partial \mathcal{E}} \Big|_{\bar{\psi}} \bar{F}_0 \right] + \frac{F(\psi)}{B_0} \langle \delta A_{\parallel g} \rangle \frac{\partial}{\partial \psi} \partial_t \bar{F}_0 \\ &\quad - c \partial_\zeta \langle \delta L_g \rangle \frac{\partial}{\partial \psi} \bar{F}_0 + [C_g + \mathcal{S}] - \frac{1}{\mathcal{J}D} \frac{\partial}{\partial \theta} \left[\mathcal{J}D \delta \dot{\theta} \delta F_z \right] \\ &\quad - \frac{1}{\mathcal{J}D} \frac{\partial}{\partial \psi} \left[\mathcal{J}D \delta \dot{\psi} \delta F_z \right] - \frac{1}{\mathcal{J}D} \frac{\partial}{\partial \mathcal{E}} \left[\mathcal{J}D \delta \dot{\mathcal{E}} \delta F_z \right] - \frac{1}{\mathcal{J}D} \frac{\partial}{\partial \theta} \left[\mathcal{J}D \delta \dot{\theta}_z \delta F \right] \\ &\quad - \frac{1}{\mathcal{J}D} \frac{\partial}{\partial \psi} \left[\mathcal{J}D \delta \dot{\psi}_z \delta F \right] - \frac{1}{\mathcal{J}D} \frac{\partial}{\partial \mathcal{E}} \left[\mathcal{J}D \delta \dot{\mathcal{E}}_z \delta F \right] - \frac{1}{\mathcal{J}D} \frac{\partial}{\partial \theta} \left[\mathcal{J}D \delta \dot{\theta} \delta F \right] \\ &\quad - \frac{1}{\mathcal{J}D} \frac{\partial}{\partial \psi} \left[\mathcal{J}D \delta \dot{\psi} \delta F \right] - \frac{1}{\mathcal{J}D} \frac{\partial}{\partial \mathcal{E}} \left[\mathcal{J}D \delta \dot{\mathcal{E}} \delta F \right], \end{aligned} \quad (21)$$

where $\dot{\mathbf{X}}_0$ denotes the gyrocenter motion in the equilibrium magnetic configuration, we have introduced the phase space variables $(\psi, \theta, \zeta, \mathcal{E}, \mu, \alpha)$, α is the gyrophase, and \mathcal{J} denotes the jacobian of the straight magnetic field line toroidal flux coordinates (ψ, θ, ζ) . Here, again, as in Eq. (19), the last three terms on the right hand side are due to symmetry breaking fluctuations only.

Equations (18) to (21) are given here without derivation, since all details and necessary in depth discussions are provided in Refs. [28, 29]. In particular, Eqs. (19) and (21) are obtained by formal manipulation of Eq. (15). Thus, they are an application of the nonlinear gyrokinetic theory and they might seem just a more convoluted way of reformulating it [4]. In order to appreciate the insights that this formal manipulation may provide, let's focus on Eq. (21) and note that \bar{F}_0 appears only in linear terms on the right had side. Recall also that \bar{F}_0 is a function of the invariants of motion in the reference magnetic equilibrium and depends explicitly on time. Furthermore, let us remind that quasineutrality equation can be obtained directly from Eq. (20) by application of equilibrium and perturbed charge neutrality, while the gyrokinetic vorticity equation is obtained by taking the moment of Eq. (21) [1, 6, 7]. Thus, we are lead to the conclusion that \bar{F}_0 is the proper choice for the definition of PSZS, once it is demonstrated that they are undamped by collisionless processes and that they evolve in time only due to nonlinear processes and/or sources and collisions [1, 2]. From Eq. (18), we can write

$$\begin{aligned} \overline{e^{iQz} \bar{F}_0} &= \overline{G_{Bz}} - \overline{e^{iQz} \delta F_z} \Big|_F + \overline{\frac{e}{m} e^{iQz} \langle \delta L_g \rangle_z \frac{\partial}{\partial \mathcal{E}} \Big|_{\bar{\psi}} \bar{F}_0} - \overline{e^{iQz} \frac{F(\psi)}{B_0} \langle \delta A_{\parallel g} \rangle_z \frac{\partial}{\partial \psi} \bar{F}_0} \\ &\equiv \overline{G_{Bz}} - \overline{\delta g_{Bz}} \Big|_S - \overline{\delta g_{Bz}} \Big|_F. \end{aligned} \quad (22)$$

Thus, that \bar{F}_0 is undamped by collisionless processes readily follows from Eq. (19). By inspection of Eq. (19), however, it can be noted that $\overline{G_{Bz}}$ is characterized by multi spatiotemporal structures, from micro- to meso- to macro-scales [1, 3, 4, 7, 31]. It seems, therefore, appropriate

to *postulate* that \bar{F}_0 is the solution of the following evolution equation

$$\begin{aligned} \partial_t \overline{e^{iQz} \bar{F}_0} &= - \overline{e^{iQz} \frac{F(\psi)}{B_0} \partial_t \langle \delta A_{\parallel g} \rangle_z \frac{\partial}{\partial \bar{\psi}} \bar{F}_0} \Big|_S - \frac{1}{\tau_b} \frac{\partial}{\partial \psi} \left[\overline{\tau_b e^{iQz} \delta \psi_z \delta F_z} \right]_S - \frac{1}{\tau_b} \frac{\partial}{\partial \mathcal{E}} \left[\overline{\tau_b e^{iQz} \delta \dot{\mathcal{E}}_z \delta F_z} \right]_S \\ &\quad - \frac{1}{\tau_b} \frac{\partial}{\partial \psi} \left[\overline{\tau_b e^{iQz} \delta \psi \delta F} \right]_{zS} - \frac{1}{\tau_b} \frac{\partial}{\partial \mathcal{E}} \left[\overline{\tau_b e^{iQz} \delta \dot{\mathcal{E}} \delta F} \right]_{zS} + \overline{e^{iQz} [C_g + \mathcal{S}]} \Big|_{zS}, \end{aligned} \quad (23)$$

with the initial condition $\bar{F}_0(\mathcal{E}, \mu, P_\phi, t = 0) = F_0(\mathcal{E}, \mu, P_\phi)$ introduced above. This equation, which can be considered as our *definition* of the PSZS by means of its dynamic evolution on the spatiotemporal meso- and macro-scales, satisfies the property of PSZS to evolve in time only due to nonlinear processes and/or sources and collisions [1, 2]. In fact, $\delta A_{\parallel z}$ is itself due to nonlinear processes as described in Eq. (14). Equation (23) is also consistent with the definition of PSZS adopted in Ref. [4] based on earlier works [3, 33]. In particular, it illuminates the concept of “neighboring nonlinear equilibria” introduced in [33], where the time evolving nonlinear equilibrium given by F_{0*} has to be understood as consisting of many neighboring equilibria, slightly deviating from the PSZS \bar{F}_0 as

$$F_{0*} \equiv \bar{F}_0 + e^{-iQz} \overline{e^{iQz} \delta F_z} \Big|_F. \quad (24)$$

The evolution equation for $\overline{e^{iQz} \delta F_z} \Big|_F$, meanwhile, is given by Eqs. (19) and (22). Thus,

$$\begin{aligned} \partial_t \overline{\delta g_{Bz}} \Big|_F &= - \overline{e^{iQz} \frac{e}{m} \partial_t \left[\langle \delta L_g \rangle_z \frac{\partial}{\partial \mathcal{E}} \Big|_{\bar{\psi}} \bar{F}_0 \right]} \Big|_F + \overline{e^{iQz} \frac{F(\psi)}{B_0} \langle \delta A_{\parallel g} \rangle_z \frac{\partial}{\partial \bar{\psi}} \partial_t \bar{F}_0} \Big|_F \\ &\quad + \overline{e^{iQz} [C_g + \mathcal{S}]} \Big|_{zF} - \frac{1}{\tau_b} \frac{\partial}{\partial \psi} \left[\overline{\tau_b e^{iQz} \delta \psi_z \delta F_z} \right]_F - \frac{1}{\tau_b} \frac{\partial}{\partial \mathcal{E}} \left[\overline{\tau_b e^{iQz} \delta \dot{\mathcal{E}}_z \delta F_z} \right]_F \\ &\quad - \frac{1}{\tau_b} \frac{\partial}{\partial \psi} \left[\overline{\tau_b e^{iQz} \delta \psi \delta F} \right]_{zF} - \frac{1}{\tau_b} \frac{\partial}{\partial \mathcal{E}} \left[\overline{\tau_b e^{iQz} \delta \dot{\mathcal{E}} \delta F} \right]_{zF}. \end{aligned} \quad (25)$$

For brevity, we omit here the equation for $\delta \tilde{g}_{Bz}$ (and, thus, $\delta \tilde{F}_{Bz}$), referring interested readers to Refs. [28, 29] for details. The nonlinear state, consisting of PSZS, \bar{F}_0 , and the fluctuations about it, $\delta \tilde{F}_{Bz}$ and $\delta \tilde{F}_{Bz}$, in the presence of the ZFS, $\delta \phi_z$, $\delta A_{\parallel z}$ and $\delta B_{\parallel z}$, and a finite level of symmetry breaking e.m. fluctuations is called the zonal state (ZS).

4. Conclusions and discussion

The theoretical framework, based on nonlinear gyrokinetic theory [8, 9, 30] and presented in this work, provides a viable route to computing fluctuation induced EP transport on long time scales in realistic tokamak plasmas and is the summary of the approach conceived and carried out by the MET project [5] and the international collaboration supporting the Center for Nonlinear Plasma Science (CNPS) [34], including the Institute for Fusion Theory and Simulation at Zhejiang University in Hangzhou [35]. The key point to emphasize is that the ZS is self-consistently computed from: (i) the solution of the linearized Eqs. (2) and (3); (ii) the solution of the NLSE-like equation for the nonlinear envelope equations, Eq. (10); (iii) the solution of Eqs. (20), (23) and (25) for the particle response averaged over linear parallel mode structures. This approach, derived from first principles and based on clear physics assumptions consistent with experimental observations [1], allows high-fidelity calculation of EP transport by reducing the dimensionality of the problem, and has been already verified/validated for energetic particle modes [2, 22], fishbones [1, 36, 37, 38], and numerous other applications [1]. As stated in Sec. 2,

this theoretical framework goes well beyond the applicability of the wave kinetic equation and of the radially local description usually adopted in flux-tube or quasilinear approaches, which can be readily recovered in the proper limits. It further improves beyond usual analyses, as it addresses transport in the phase space; and allows the ZS to significantly deviate from the result generally assumed by balancing sources and collisions. As argued in Refs. [4, 28, 29], this is of crucial importance for computing transport self-consistently on long time scales, in particular for collisionless EPs. The generality of the present approach does not restrict its applicability to nonlinear gyrokinetic theory: it can be applied to any nearly integrable Hamiltonian system, provided the fundamental field equations are known [4]. Furthermore, given the introduction and detailed analysis of the concept of “neighboring nonlinear equilibria” [33], this approach provides a novel interpretation of why and how “ensemble averaging” [30, 39] and “time averaging” [4, 28, 29] among different realizations of the ZS should be consistent. In other words, this work addresses the equivalence of “statistical” and “ab initio” approaches to plasma transport. The applicability of the present approach not only to EP [29] but thermal plasma transport as well is shown in Refs. [4, 28]. In particular, it is possible to show that radial transport described within this framework reduces to well-known expressions adopted in the literature (cf. *e.g.*, Ref. [30]), when evolution of plasma profiles on the macro-scales are considered [4].

The present theoretical framework is also well-suited for the construction of first-principle based (further) reduced models [5, 34]. The existence of a good asymptotic expansion parameter, $|\omega_n| \tau_{NLn} \gg 1$ (cf. Sec. 2), suggests using a weak-field expansion based on diagonal interactions [40, 41, 42, 43, 44, 45, 46, 47] for obtaining explicit expressions of EP fluxes in the phase space, including resonance broadening [44], nonlocal behaviors, EP avalanches and fast convective particle redistributions [1, 2, 48]. These issues are dealt with in detail in Ref. [29]. Here, we merely remind interested readers that EP induced avalanches, described in this way, consist of convectively amplified radially propagating solitons, which are accompanied by secular radial transport [1, 2, 3, 22]. Similar radial spreading due to soliton formation is observed in the nonlinear interaction of ion temperature gradient driven turbulence and ZFS [26]. When reduced to diagonal interactions, the nonlinear radial envelope equations can be describe in term of the nonlinear distortion of the ZS only, that is by F_{0*} in Eq. (24), which provides the *renormalization* of EP response [1, 2, 3, 4], since it accounts for the modification of the reference EP distribution function to compensate for effects that are due to nonlinear plasma behaviors (self-interactions). Equations (23) to (25) can then be cast in the form of a *Dyson-like equation* [49, 50], which can be solved for the renormalized ZS and formally represented as Dyson series [1, 2, 3]. EP fluxes in phase space can then be expressed in a compact form [48] that will be reported in Ref. [29] and constitute the foundation of the reduced Dyson Schrödinger transport Model (DSM).

Acknowledgments

This work was carried out within the framework of the EUROfusion Consortium and received funding from Euratom research and training programme 2014–2018 and 2019–2020 under Grant Agreement No. 633053 (Project No. WP19-ER/ENEA-05). The views and opinions expressed herein do not necessarily reflect those of the European Commission. This work was also supported by Fundamental Research Fund for Chinese Central Universities (No. 2019FZA3003).

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