Thermodynamic Constraints Applied to Tokamaks

Using gyrokinetic equations, it is shown that, for collisionless plasmas, the largest source of kinetic free energy in tokamaks is expansion energy coming from the parallel temperature. Expansion energy is independent of the current, but collisional flows may add current-dependent free-energy sources. Even so, an upper bound on drift-wave growth rates derived from free energy is independent of the current.

Key Words: *free energy, gyrokinetic equations, bounds on growth rates, fluctuations, tokamaks*

This paper applies the free-energy method to obtain nonlinear upper bounds on fluctuations and upper bounds on linear growth rates in tokamaks.[1] The ultimate goal is to obtain estimates of transport based on thermodynamic constraints rather than the explicit evolution of the system in time. Here we give a progress report citing a few new results and discuss the potential and limitations of the method.

Whereas Ref. 1 employed the full Maxwell–Vlasov equations, we have reformulated the method for gyrokinetic equations applicable to drift waves. For simplicity, we consider only electrostatic potential fluctuations, though the extension to the fully electromagnetic case is straightforward.[2]

The nonlinear gyrokinetic Vlasov–Poisson equations and their associated invariant energy functional $\mathscr{E}$ have been derived previously.[3] It is straightforward to show that these equations also

Comments Plasma Phys. Controlled Fusion
1991, Vol. 14, No. 5, pp. 263–273
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conserve the particle number $\mathcal{N}$ and, in the absence of collisions, the entropy $\mathcal{S}$. Using these results, we can construct the gyrokinetic Gibbs free energy, of the form $\mathcal{E} - T\mathcal{S} - T\mathcal{N}$, that is an exact invariant of these equations. An approximate form of this invariant sufficient for our purposes is given by

$$\begin{aligned} \mathcal{A}_{gy} &= \sum_\sigma \int d^5 Z F \left[\epsilon + T\left(\ln \frac{F}{C} - 1 \right) \right] + \int d^3 r \frac{\epsilon_0}{8\pi} |\nabla_\perp \phi|^2 \\ &\equiv \mathcal{H}[F] + \Phi, \end{aligned} \tag{1}$$

where Φ is the electrostatic energy term on the right and $\mathcal{H}$ denotes the remainder. The distribution $F(\mathbf{X}, \epsilon, \mu, t)$ is a function of the *gyrocenter* particle energy ϵ, the *gyrocenter* magnetic moment μ, and the guiding-center position $\mathbf{X}$; $d^5 Z = \mathcal{J}\, d\epsilon d\mu d^3 X$, where $\mathcal{J} = (2\pi B/m^2)\,[2(\epsilon - \mu B)/m]^{-1/2}$ and B is the magnetic field; C and T are constants to be determined; and ϕ is the electrostatic potential fluctuation (we neglect ϕ_0) which satisfies

$$- \nabla_\perp \cdot \epsilon_0 \nabla_\perp \phi(\mathbf{X}, t) = 4\pi \sum_\sigma e \int \mathcal{J} d\epsilon d\mu F(\mathbf{X}, \epsilon, \mu, t), \tag{2}$$

where Σ_σ sums over particle species and $\sigma = \pm 1$ depending on the sign of the parallel velocity component.

To obtain these simple results from the complex expressions in Refs. 3 and 4, we have taken advantage of the fact that F is never far away from a Maxwellian state and replaced F by $F_M = C\exp(-\epsilon/T)$ in terms multiplied by ϕ, since $e\phi/T \ll 1$ in gyrokinetics. Also, we have expanded $\phi(\mathbf{r})$ and the gyrokinetic Jacobian $\mathcal{J}$ in powers of the gyroradius vector $\boldsymbol{\rho} = \mathbf{r} - \mathbf{X}$, keeping only lowest-order terms. Omitted terms are order ρ/L, where L is the shear length, curvature radius, plasma minor radius, etc. Note the explicit appearance of a dielectric constant ϵ_0, where $(\epsilon_0 - 1)$ represents $E \times B$ motion ($\epsilon_0 = 1 + c^2/v_A^2$, with the Alfvén velocity v_A evaluated at $\mathbf{X}$).

We are now in a position to obtain an upper bound on the fluctuation energy, $\Phi(t)$, valid for all time. Initially let $F = F_0 + f$, where F_0 is the equilibrium distribution and f is an infinitesimal perturbation, and $\Phi(0) \cong 0$. Since $\mathcal{A}_{gy}$ is conserved, at a later time $\Phi(t) - \Phi(0) \cong \Phi(t) = \mathcal{K}[F_0] - \mathcal{K}(t) + \mathcal{O}(f)$. Following Ref. 1, we obtain a bound by replacing $\mathcal{K}(t)$ by its minimum value for any state conserving $\mathcal{N}$ and $\mathcal{S}$, which occurs for the Maxwellian distribution $F_M = C_M \exp(-\epsilon/T_M)$ with Lagrange multipliers (C_M, T_M) chosen so that F_0 and F_M have the same $\mathcal{N}$ and $\mathcal{S}$. Then $\Phi(t) \leq \mathcal{K}[F_0] - \mathcal{K}[F_M]$, now discarding terms $\mathcal{O}(f)$. Using Eq. (1) this becomes

$$\Phi(t) \leq \sum_\sigma \int d^5Z \epsilon(F_0 - F_M) \cong \sum_\sigma \int d^5Z \frac{T_M(\Delta F)^2}{2F_M}. \quad (3)$$

The first expression (just the change in kinetic energy) equals $\mathcal{K}[F_0] - \mathcal{K}[F_M]$ exactly since $\mathcal{N}$ and $\mathcal{S}$ are held constant. The second expression is obtained by expanding $\mathcal{K}[F_0]$ in powers of $\Delta F = F_0 - F_M$, assumed small since F_0 cannot be far from a Maxwellian in a device with good confinement.

Still following Ref. 1, we apply the bound locally. That is, we restrict attention to a shell of average thickness equal to the maximum perpendicular wavelength of interest (denoted by k^{-1}) centered on a particular flux surface. In taking $\mathcal{A}_{gy}$ constant, we neglect free-energy flows into or out of this shell. Let $F_0 = \bar{F}_0(1 + \alpha)$, where $\bar{F}_0$ is a spatially uniform Maxwellian with density $\bar{n}$ and temperature $\bar{T}_0$ averaged over the shell, and $N = \int d^3X\, n(\mathbf{X})$ within the shell. Then, to conserve particles and entropy, we require

$$C_M = \left(\frac{m}{2\pi\bar{T}_0}\right)^{3/2} (1 + \bar{\alpha})$$

and

$$T_M = \bar{T}_0 \left[1 - \frac{1}{3}\overline{(\alpha - \bar{\alpha})^2}\right], \quad (4)$$

to lowest order in α and $\bar{\alpha}$. The overbar denotes a phase-space average with weighting factor $N^{-1}\exp(-\epsilon/\bar{T}_0)$. Substituting these expressions into either form of Eq. (3) gives the bound

$$\Phi \cong \frac{1}{8\pi}\int d^3X\epsilon_0|\nabla_\perp\phi|^2 \leq \sum_\sigma \frac{N\bar{T}_0}{2}\overline{(\alpha - \bar{\alpha})^2}. \tag{5}$$

We first apply the bound to collisionless equilibria in the toroidal rest frame, taking $F_0 \propto (n/T_0^{3/2})\exp(-\epsilon/T_0)$, where n and T_0 are functions of $\mathbf{X}$. Let x be the displacement about the chosen flux surface. Expanding in x gives

$$\alpha(\epsilon, x) = x\left[\frac{n'}{\bar{n}} + \frac{T_0'}{\bar{T}_0}\left(\frac{\epsilon}{\bar{T}_0} - \frac{3}{2}\right)\right], \tag{6}$$

and substituting this into Eq. (5) gives, for $T_i = T_e$,

$$\Phi \leq \frac{N\bar{T}_0}{12k^2L_n^2}\left(1 + \frac{3\eta^2}{2}\right), \tag{7}$$

where $\eta = L_n/L_T$ and $L_n = |\bar{n}/n'|$, $L_T = |\bar{T}_0/T_0'|$, in usual notation. This is the familiar expansion energy[1] released when the initially nonuniform plasma expands to fill the shell uniformly (like expansion cooling of a gas).

Two new features of the gyrokinetic formulation are the explicit appearance in Φ of the dielectric constant ϵ_0, as already noted, and a demonstration that the largest reservoir of free energy available to drive drift waves is the parallel temperature, both being consequences of *gyrocenter* magnetic moment conservation. The second point is obvious in a uniform magnetic field, since the perpendicular kinetic energy cannot change ($\Delta\mathcal{K}_\perp = 0$). However, the parallel energy can change even though the pressure is initially uniform along field lines. Physically, if $k_\parallel \neq 0$, radial $E \times B$ motion is spatially varying in sign along field lines, which creates parallel pressure gradients that release parallel energy by expansion along the field lines.

For a tokamak plasma, $\Delta\mathcal{K}_\perp \propto n'B'$ is smaller than the expansion energy ($\propto n'^2$) by an aspect ratio, so again most of the energy must come from the change in parallel kinetic energy $\Delta\mathcal{K}_\parallel$. Moreover, contrary to a conjecture made in Ref. 1, even a very large change in $\Delta\mathcal{H}_\perp$ cannot overcome the expansion energy allowed by the conservation of entropy. Rather, $\Delta\mathcal{H}_\parallel$ is allowed to compensate for $\Delta\mathcal{H}_\perp$. This can be seen directly by rewriting Eq. (1) using $\Delta\mathcal{H}$ from Eq. (5) in the form $\int d\mu N_\mu \bar{T}_0 \overline{(\alpha - \bar{\alpha})^2_\mu}$, where the μ-integration has not yet been carried out (so that N_μ and α may still depend on μ). In other words, $\Delta\mathcal{H}$ is the sum of expansion free energy separately for each value of μ. But since entropy and particle number are conserved separately for each value of μ, this can only be true if $(\Delta\mathcal{H}_\parallel)_\mu = (\text{Expansion})_\mu - (\Delta\mathcal{H}_\perp)_\mu$. This can be verified directly by carrying out the variation of $\mathcal{A}_{gy}$ before integrating over μ, whereby C_M and T_M can depend on μ, and calculating $(\Delta\mathcal{H}_\parallel)_\mu$ with C_M and T_M expanded to higher order in α.

We turn now to bounds on the linear growth rates, derived from the time derivative of the quadratic expression obtained by expanding $\mathcal{A}_{gy}$ in powers of the perturbation $f = F - F_0$, given by

$$\mathcal{A}_2 = \sum_\sigma \int d^5Z \frac{Tf^2}{2F_0} + \int \frac{d^3X}{8\pi} \epsilon_0 |\nabla_\perp \phi|^2 \equiv \mathcal{H}_2 + \Phi_2. \qquad (8)$$

While the kinetic term is formally similar to Eq. (3), note that Eq. (3), expanded about the extremal *final* state F_M, gives fully nonlinear results, while $\mathcal{A}_2$, expanded about the *initial* state F_0, will give linearized growth rates. Regarding f as f_1 in a formal expansion $F = F_0 + f_1 + f_2 + \cdots$, the sum of $\mathcal{A}_2$ and the corresponding second-order functional of f_2 would be conserved to second order,[2] but $\mathcal{A}_2$ alone is not conserved by the linearized equations, as follows.

Using the linearized gyrokinetic Vlasov–Poisson equations, we can show that

$$\frac{d\mathcal{A}_2(t)}{dt} = \sum_\sigma e \int d^5Z f(\mathbf{X}, \epsilon, \mu, t) \nabla_\perp \phi(\mathbf{X}, t) \cdot \mathbf{u}_\perp(\mathbf{X}, \epsilon, \mu), \qquad (9)$$

where $\mathbf{u}$ is the unperturbed fluid velocity (including diamagnetic drift, parallel flows, etc.). For α in Eq. (6), we find to lowest order in α and ρ,

$$u_\perp = \frac{c\bar{T}_0}{eB}\frac{\partial\alpha}{\partial x} = \frac{c\bar{T}_0}{eB}\left[\frac{n'}{\bar{n}} + \frac{T_0'}{\bar{T}_0}\left(\frac{\epsilon}{\bar{T}_0} - \frac{3}{2}\right)\right], \tag{10}$$

where we only retain the component perpendicular to the equilibrium magnetic field, since for the low-frequency drift waves, $u_\| E_\| << u_\perp E_\perp$, although in tokamaks $u_\| > u_\perp (u_\| E_\| / u_\perp E_\perp = \mathcal{O}(\rho/L_n))$. Note that all effects due to magnetic-field nonuniformity (i.e., gradient, curvature, or shear) have dropped out as they are smaller by $\mathcal{O}(\rho/L)$.

Again following Ref. 1, γ is bounded by the logarithmic time derivative of $\mathcal{A}_2$, maximized for any perturbation:

$$\gamma \leq \left(\frac{1}{2\mathcal{A}_2}\frac{d\mathcal{A}_2}{dt}\right)_{\max} \leq \sum_\sigma \frac{\|u_\perp\|}{\lambda_D \epsilon^{1/2}}, \tag{11}$$

where ϵ is defined below and λ_D is the Debye length. As in Eq. (10), $u_\perp$ may contain several terms $u_{\perp l}$ with $\|u_\perp\| = \Sigma_l \|u_{\perp l}\|$, where $\|u_{\perp l}\| \equiv [(\overline{u_{\perp l}^2})_{\max}]^{1/2}$ is the rms velocity average of $u_{\perp l}$ (with overbar as previously defined) and here max refers to extreme values at any position x within the integration volume. Using Eq. (9) to calculate $d\mathcal{A}_2/dt$ yields Eq. (11) after applying successive Schwarz inequalities as described in Ref. 1.

The perturbations f and ϕ appear only through the dielectric constant ϵ, defined by

$$\epsilon = \frac{\epsilon_0}{R}(R^2 + 1), \tag{12}$$

where $R \equiv \mathcal{H}_2/\Phi_2$. A similar expression was found in Ref. 1 without the factor ϵ_0 (i.e., the full Vlasov case), and it was noted that the minimum value is $\epsilon_{\min} = 4$. For the gyrokinetic case, we have $\epsilon_{\min} = 4\epsilon_0 >> 4$. In Table I, we identify these minima in ϵ with high-frequency drift-cyclotron waves[5] for the full Vlasov system (recall that we dropped $u_\|$), and MHD interchange for the gyrokinetic case ($\omega_D \sim (a/R)^{1/2}\omega_*$ is the curvature drift frequency). We now

TABLE I

Comparison of bounds and actual values for electrostatic growth rates

Modes	ϵ	γ Bound	Actual γ
Drift-cyclotron ($k\rho_i \ll 1$)	~ 1	$\sim \omega_*/k\lambda_D$	$\sim (k\rho_i)^{-1/2}\omega_* k\lambda_D$
Interchange	$\sim \epsilon_0$	$\sim \omega_*/k\rho_i$	$\sim (\omega_*\omega_D)^{1/2}/k\rho_i$
Drift waves	$\sim (k^2\lambda_D^2)^{-1}$	$\sim \omega_*$	$\sim \omega_*$

show that ϵ also has a finite maximum, which we shall identify with drift waves.

Using Poisson's equation to relate f and ϕ, we rewrite $\Phi_2 = \frac{1}{2} \Sigma \int ef\phi$ and vary ϵ with respect to f. Then $\delta\epsilon \propto (1 - R^{-2})\delta R$ indicates a minimum at $R = 1$ (as noted above), while setting $\delta R = 0$ gives

$$\delta R = 0 = \frac{1}{\Phi_2} \sum_\sigma \int d^5 Z \delta f \left(f \frac{T_0}{F_0} - e\phi R \right), \qquad (13)$$

from which extrema occur if

$$f = R \frac{e\phi}{T_0} F_0. \qquad (14)$$

Substituting this f in Poisson's equation gives

$$-\nabla_\perp \cdot \epsilon_0 \nabla_\perp \phi = R \sum_\sigma \int \mathcal{J} d\epsilon d\mu \frac{4\pi e^2 F_0}{T_0} \phi = R \sum \frac{\phi}{\lambda_D^2}. \qquad (15)$$

This is an eigenvalue problem in R that selects out different classes of perturbations (different wavenumbers, k). In the local approximation, $\nabla_\perp^2 \to -k^2$ (although exact expressions are attainable). Then for $T_i = T_e$, we find $R = (k^2\lambda_D^2/2)\,\epsilon_0$, from Eq. (15), which gives by Eq. (12) a minimum $\epsilon_{min} = 4\epsilon_0$ at $R = 1$ ($k\rho_i \sim 1$) and a maximum at $R \ll 1$ ($k\lambda_D \ll k\rho_i \ll 1$),

$$\epsilon_{max} \to \frac{2}{k^2\lambda_D^2}. \qquad (16)$$

That this is indeed a maximum can be shown by evaluating $\delta^2\epsilon$ directly; the critical step is to show, by Schwarz inequality on the double sum $\Sigma \int$, that $R(4\pi k^{-2})\,(\Sigma \int \delta f)^2 \leq \Sigma \int \delta f^2(T/F_0)$ at $\delta R = 0$.

Note that Eq. (16) and the corresponding bound on γ, by Eq. (11), are identical with corresponding results for the full Vlasov case, discussed in detail in Ref. 6. This is true because Eqs. (9)–(16), correct to $\mathcal{O}(\rho/L)$ for gyrokinetics, become the corresponding exact equations for the full Vlasov–Poisson system if we simply set $\epsilon_0 = 1$ whenever i appears. Thus ϵ_{max} is the same for both theories.

Identifying ϵ_{max} with drift waves is conjectural but reasonable. Note that substituting an exact solution f into $\mathcal{A}_2$ in Eq. (11) would give γ exactly. Our extremal f, Eq. (14), is in fact the leading adiabatic term valid if $\omega << k_{\|}v$, as is true of electrons in drift waves and marginally so for the ions. (For MHD, with $\omega > k_{\|}v$, the adiabatic term cancels.) Making this conjecture, Eq. (11) gives, for α in Eq. (6) and $T_i = T_e$,

$$\gamma_{DW} \leq \sum_{\sigma} \frac{ck\bar{T}_0}{\sqrt{2}eB} \left\| \frac{\partial \alpha}{\partial x} \right\| = \sqrt{2}\omega_* \left(1 + \sqrt{\frac{3}{2}}\,\eta\right), \qquad (17)$$

where $\omega_* = ck\bar{T}_0/eBL_n$, and the subscript DW denotes electrostatic instabilities to which the gyrokinetic ordering applies (e.g., drift waves, trapped-particle modes, etc.).

With this interpretation, Table I shows that both our bound and the actual growth rates form a hierarchy in which growth rates decrease as ϵ increases. The drift waves are the lowest-lying family of γ's in this hierarchy, corresponding to the maximum, adiabatic dielectric constant.

We have applied our bound on γ, Eq. (17), to calculate a mixing-length estimate of transport coefficients, of the form $\chi = \gamma/k^2$. Recent calculations have demonstrated fair agreement between global energy confinement times in tokamaks and estimates based on radial averages of $\chi \nabla T$, with χ of the above form and approximate formulas for γ for ion temperature gradient (ITG) modes and dissipative trapped-electron (DTE) modes.[7] For the same k, our bound on γ gives approximately the same results as these growth rates, and therefore similar estimates of the global energy confinement time. We have compared our $\chi = \gamma/k^2$, taking γ from Eq. (17), with the corresponding quantity, $\chi = (5/2k^2)(2\gamma_{\mathrm{DTE}} + \gamma_{\mathrm{ITG}}/2)$, found to fit the experimental data on confinement times in Ref. 7 (the factors 2 and 1/2 having been adjusted to provide a best fit). We find close agreement at all radii (perhaps fortuitously), our χ being about 25% higher. However, our method cannot yet determine the worst k, for which we took $k\rho_i = 1/3$, approximately the value used in Ref. 7.

Our nonlinear bound on fluctuations supports the mixing-length estimate in that δE allowed by Eq. (7) ($\delta E \leq (k\rho_i)^{-1}(T/eL_n)$) is more than sufficient to flatten the profile in one cycle ($\omega^{-1}\,\delta E/B \geq k^{-1}$ if $\omega = \omega_*$ and $k\rho_i < 1$). In fact δE at saturation would be just that needed to flatten the profile if, instead of ϵ_0, the dielectric constant were replaced by $\epsilon \sim (k^2\lambda_D^2)^{-1}$ as suggested by the linear theory, Eq. (16). Then $\delta E \sim T/eL_n$ and $\omega_*^{-1}\,\delta E/B = k^{-1}$.

That our method does not yet determine the worst k (or mixing length) is a serious defect. Further progress requires constraints not included in the free energy functional, which is not sensitive to shear or other subtleties of magnetic geometry, and does not exhibit Landau damping (in which $\mathcal{H}$ increases as Φ decreases). Earlier efforts to incorporate such effects did not succeed.[1] However, the fact that more recent experimental evidence, such as that cited above, generally supports the thermodynamic estimate of χ now encourages us to try again. In some sense, we have disected χ into three parts: u, ϵ, and k. Two of these parts, u and ϵ, appear to be determined mainly by global thermodynamic constraints. It remains to isolate the constraints that fix k.

Like other drift-wave calculations, our mixing-length estimate and also our nonlinear bound on fluctuations fail to exhibit the strong dependence on current that characterizes empirically determined energy confinement times in tokamaks.[7] Nor is it obvious that further refinements of the present calculations (flux surface averages, etc.) would disclose a current dependence. Perhaps free-energy sources other than expansion are involved.

Our formulation is easily extended to include other free-energy sources in F_0, all such effects representing small departures from a Maxwellian that contributes additively to α. Again bounds on Φ and γ can be calculated by substituting the new α into Eqs. (5)

and (17). Examples are parallel collisional flows, arising in neoclassical MHD theory, which do depend on the current and which dominate over the expansion energy in the bound on Φ for wavelengths typical of drift waves.[8] However, these effects do not significantly alter $\partial\alpha/\partial x$ and hence they do not affect our bound on γ. In that case, the mixing-length estimate tying saturation to γ may be questionable. A different estimate is $\tau_E \sim \int d^3X\, nT/P_V$, where P_V is the transient flow of free energy across the chosen flux surface. Following Ref. 1 (Section IV), we estimate $P_V \sim \gamma\Delta\mathcal{H}$, yielding

$$\tau_E \sim \frac{\int d^3X\, n\bar{T}_0}{\gamma\Delta\mathcal{H}} \sim \frac{2}{\gamma\overline{(\alpha - \bar{\alpha})^2}}. \tag{18}$$

For expansion energy ($\alpha \sim (k^2L_n^2)^{-1}$) this again yields the mixing-length estimate. For collisional flows, $\alpha \sim \Delta x/L_T$, where $\Delta x \sim q\rho_i/(a/R)^{1/2}$ (with safety factor $q \propto B/I$ and current I) is the banana width.[8] Then $\tau_E \sim 2L_T^2/\gamma\Delta x^2$. This is smaller than τ_E from the mixing-length estimate if $k\Delta x > 1$ (true for $k\rho_i \sim 1/3$ as assumed above and typical $q \sim 3$) and happens to scale as $\tau_E \sim I^2$, as does the empirical law $\tau_E \sim I/\sqrt{P}$ with $P = \int d^3X\, n\bar{T}_0/\tau_E$.

Acknowledgment

This work was performed under U.S. DOE contracts DE-FGO3-89ER5116 and DE-FGO5-80ET-53088.

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Received July 17, 1991
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