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GYROKINETIC SIMULATION OF ISOTOPE SCALING
IN TOKAMAK PLASMAS

BY

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Gyrokinetic Simulation of Isotope Scaling in Tokamak Plasmas

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A three-dimensional global gyrokinetic particle code in toroidal geometry has been used for investigating the transport properties of ion temperature gradient (ITG) drift instabilities in tokamak plasmas. Using the isotopes of hydrogen (H^+), deuterium (D^+) and tritium (T^+), we have found that, under otherwise identical conditions, there exists a favorable isotope scaling for the ion thermal diffusivity, i.e., χ_i decreases with mass. Such a scaling, which exists both at the saturation of the instability and also at the non-linear steady state, can be understood from the resulting wavenumber and frequency spectra.

The agreement between the recent beam emission spectroscopy and microwave reflectometry measurements of the density fluctuations for the supershot discharges in TFTR^{1,2} and the 3D gyrokinetic particle simulation of the ion temperature gradient (ITG) drift instability³ have not only shown the importance of microturbulence for tokamak confinement but also pointed out the dominant role assumed by the long wavelength ($k_{\perp}\rho_i < 1$) fluctuations. In this paper, we report on the investigation concerning the effects of these long wavelength modes on transport scaling. More specifically, we have used various hydrogenic isotopes (H^+ , D^+ , and T^+) in the microturbulence simulation to study the trend for mass scaling and, in turn, to obtain some physical insight concerning the mechanisms responsible for anomalous transport.

Briefly, our simulation results give a favorable mass dependence for χ_i . Although these simulations have been carried out under most idealized conditions and do not contain all the physics of realistic tokamak discharges, they do contain what we believe to be some of fundamental physics of tokamak plasmas. Therefore, it is not surprising that our mass scaling results are in qualitative agreement with the experimental trend observed in most of the existing tokamaks.⁴ However, the observed mass dependence is not as strong as the latest analyses from the D-T discharges in TFTR.⁵ In the nonlinear steady state of the simulation, two important physical characteristics related to the scaling have been identified: the widths for both the radial wavenumber spectra and the frequency spectra decrease with mass. The significance of these observations will be discussed.

In the simulation, we have used the δf scheme for particle pushing,^{6,7}

for which the original equations of motion for the ion gyrocenters⁸ in the gyrokinetic unit of $\rho_s (\equiv \sqrt{T_e/T_i} \rho_i)$ and $\Omega_i (\equiv c_s/\rho_s)$ and $c_s (\equiv \sqrt{T_e/m_i})$ without the nonlinear parallel acceleration can be written as

$$\dot{\mathbf{R}} \equiv \frac{d\mathbf{R}}{dt} = U\hat{\mathbf{b}}^* + \mu\hat{\mathbf{b}} \times \frac{\partial}{\partial \mathbf{R}} \ln B + \hat{\mathbf{b}} \times \frac{\partial \bar{\phi}}{\partial \mathbf{R}}, \quad (1)$$

$$\dot{U} \equiv \frac{dU}{dt} = -\hat{\mathbf{b}}^* \cdot \mu \frac{\partial}{\partial \mathbf{R}} \ln B, \quad (2)$$

and $\mu/B \equiv v_\perp^2/2B = \text{const.}$, where $\hat{\mathbf{b}}^* = \hat{\mathbf{b}} + U\hat{\mathbf{b}} \times (\hat{\mathbf{b}} \cdot \partial/\partial \mathbf{R})\hat{\mathbf{b}}$ and $\bar{\phi}(\mathbf{R})$ is the finite Larmor radius (FLR) modified potential in unit of e/T_e .⁹ The “weight” of the particle is given by

$$\dot{w} \equiv \frac{dw}{dt} = -\kappa \frac{\partial \bar{\phi}}{\partial \mathbf{R}} \times \hat{\mathbf{b}} \cdot \hat{\mathbf{r}} - \frac{T_e}{T_i} U \hat{\mathbf{b}}^* \cdot \frac{\partial \bar{\phi}}{\partial \mathbf{R}}, \quad (3)$$

where $\kappa = \kappa_n - (3/2 - v^2/2v_i^2)\kappa_T$ and $\hat{\mathbf{r}}$ is the unit vector in the minor radius direction. The corresponding δf becomes

$$\delta f = \sum_{j=1}^N w_j \delta(\mathbf{R} - \mathbf{R}_j) \delta(\mu - \mu_j) \delta(U - U_j), \quad (4)$$

where N is the total number of particles in the simulation. Thus, we are solving the equation

$$(\partial/\partial t + \dot{\mathbf{R}} \cdot \partial/\partial \mathbf{R} + \dot{U} \partial/\partial U) \delta f = \dot{w} f_M \quad (5)$$

in the simulation, where the background Maxwellian f_M is spatially homogeneous. With the assumption that the electron response is adiabatic, i.e., $\delta n_e/n_0 \approx \phi(\mathbf{x})$, where n_0 is the average number density, the gyrokinetic Poisson equation in the Fourier $\mathbf{k}$ space takes the form of

$$[1 + (T_e/T_i)(1 - \Gamma_0(b_i))]\phi(\mathbf{k}) = \delta \bar{n}_i(\mathbf{k})/n_0, \quad (6)$$

where $\Gamma_0 = I_0(b_i)\exp(-b_i)$, I_0 is the modified Bessel function and $b_i \equiv (k_\perp \rho_i)^2$. $\delta \bar{n}_i$ is the perturbed number density, $\int \delta f_i dU d\mu$, modified by the FLR effects.⁹ The ion thermal diffusivity in the δf representation can be written as⁹

$$\chi_i = \frac{1}{\kappa_{Ti} + \kappa_n} \sum_{j=1}^N -\frac{U_j^2 + 2\mu_j}{v_{ti}^2} w_j \left. \frac{\partial \bar{\phi}}{\partial \mathbf{R}} \right|_{\mathbf{R}_j} / 3N. \quad (7)$$

The simulation has been carried out on a 128x128x64 toroidal grid [a “square” torus model in $(x, y, -R_0\varphi)$ coordinates³] with 4.2×10^6 ion gyrocenters (or particles). The toroidal and poloidal magnetic fields are given by $B_t = B_0/(1 + x/R_0)$ and $B_p = rB_0/qR$, respectively, where $q = q_0 + [q_a - q_0](r/a)^2$. The ion temperature gradient is represented $\kappa_{Ti} = (1/L_{Ti0})\text{sech}^2(r - r_0/L_w)$, where the maximum is located at r_0 and L_w is the width of the region with active drive. In the gyrokinetic units of $\rho_s D$ and Ω_D^{-1} (i.e., ρ_s and Ω_i^{-1} for the deuterium ions), the other relevant simulation parameters are: $a = 100$, $R_0 = 1000$, $q_0 = 1$, $q_a = 3$, $L_w = 30$, $r_0 = 55$, $T_e/T_i = 1$, L_n (density scale length) $\equiv 1/\kappa_n = \infty$, and $L_{Ti0} = 100$, $\Delta t = 30$ and $t_{tot} = 150000$.

The time history of the ITG instability in terms of the gyrokinetic electrostatic field energy,⁹ $\sum_k [1 - \Gamma_0(b_i)] (T_e/T_i) |e\phi/T_e|^2$, for all three ion species is shown in Fig. 1(a). It clearly shows four different stages of the evolution: linear growth, nonlinear saturation, transition period and steady state. In the linear stage, the trend for the mass dependence of growth rates is consistent with the prediction of $\gamma_L \sim 1/\sqrt{M}$ by Dong et al.¹⁰ The nonlinear saturation level in Fig. 1(a) seems to track the linear growth and, in turn, has similar mass dependence. After a period of transition, in which the mass

dependence is reversed, the original trend is again restored in the steady state, where the fluctuating field energy stays roughly constant. Figure 1(b) gives the measured ion thermal diffusivity for all three ion species. It has a mass dependence similar to that of the field energy. In this paper, we will focus on the scaling trend at saturation and at steady state.

To understand the physics for the observed isotope scaling, let us first study the radial wavenumber spectra taken at the linear stage just before the saturation as shown in Fig. 2(a). The dominant modes are $m \approx 16, 13, 11$ for H^+ , D^+ , and T^+ , respectively, and are characterized by their ballooning structures.³ This is the period where k_r is at its minimum. Using the full width half maximum (FWHM) as the reference point, one can see the $k_r \sim 1/M^{1/4}$ dependence for the three species. This is in agreement with the theoretical predictions for the long wavelength toroidal instabilities that the radial structures are prescribed by the equilibrium profile¹¹ (i.e., L_w in our case) and that, near the maximum gradient, the radial mode widths are proportional to $\rho_i^{1/2} (\sim M^{1/4})$.^{12,13} However, near the time of saturation and shortly afterwards, there is a breakup of these spatially coherent structures and the corresponding FWHM wavenumbers become more than doubled. During the ensuing transition period, large amplitude oscillations in k_r take place between these two extremes. In the steady state, the amplitude settles to around $\Delta k_r \approx 0.1 \rho_{sD}^{-1}$ for $0 \leq k_r \leq 0.5 \rho_{sD}^{-1}$ and the time-averaged radial wavenumber spectra are shown in Fig. 2(b). Here, the mass dependence for the FWHM wavenumber changes to $k_r \sim 1/M^{1/2}$ with $k_r \rho_s \approx 0.3$. In addition to the active modes observed in the linear stage, lower toroidal harmonics of $m \approx 12, 9, 7$ for H^+ , D^+ , T^+ , respectively, have also been

excited. The corresponding time-averaged k_θ and k_ϕ spectra are shown in Figs. 3(a) and (b), respectively. Unlike the k_r spectra, the poloidal and toroidal wavenumbers don't oscillate much in time in the nonlinear stage. However, all three spectra have the same property, i.e., $k_r \rho_s$, $k_\theta \rho_s$ (≈ 0.15) and $k_\phi \rho_s$ ($\approx 0.6 \times 10^{-2}$) are all nearly invariant for all three species, where $\rho_s \sim \sqrt{M}$. Another interesting diagnostic is the frequency spectra in the second half (nonlinear steady state) of the simulation. Figure 4 shows the spatially averaged spectra along the weak field side of the midplane at a fixed toroidal angle for H^+ , D^+ , and T^+ plasmas. The results indicate that the nonlinear frequency decreases with mass and, interestingly, so does the frequency spread, $\Delta\omega$. This important property is vital for the understanding of the observed scaling, which we will discuss.

To fully understand the results presented here, one needs a self-consistent nonlinear theory, which is beyond the scope of the present paper. Short of that, let us compare them with some of the present understanding of turbulent transport, e.g., the mixing length argument which gives the scaling of $\chi_i \sim \gamma_L/k_\perp^2$. Since $\omega_{*Ti}/\Omega_i = k_\theta \rho_s^2/L_{Ti}$, one can argue that $\gamma_L/\Omega_i \approx \rho_s/L_{Ti} \sim \sqrt{M}$, if $k_\theta \rho_s$ is invariant. This mass dependence is in agreement with the calculation by Dong et al.,¹⁰ which also shows that most unstable toroidal ITG modes occur at $k_\theta \rho_s \approx 0.5$. Thus, we obtain the familiar expression of

$$\chi_i \sim \frac{\rho_s/L_{Ti}}{(k_r \rho_s)^2} \frac{cT_e}{eB}. \quad (8)$$

Here, the use of the radial wavenumber k_r for the diffusion can be justified from the quasilinear theory (see, e.g., Ref. 14). This scaling can also be obtained from a set of gyrofluid equations based on a simplified Eq. (5) with

$\dot{\mathbf{R}} \approx U \hat{\mathbf{b}}^* \cdot \hat{\mathbf{y}} + \hat{\mathbf{b}} \times \partial \phi / \partial \mathbf{R}$, $\dot{U} \approx 0$, $\dot{w} \approx -\kappa \partial \phi / \partial y - (T_e/T_i) U \hat{\mathbf{b}}^* \cdot \partial \phi / \partial \mathbf{R}$, $\hat{\mathbf{b}}^* \approx \hat{\mathbf{b}} - (U/R_0) \hat{\mathbf{y}}$, and $\kappa \approx \kappa_n - (1 - U^2/v_{ti}^2) \kappa_{Ti}/2$, where $\hat{\mathbf{b}}$ is in the toroidal direction only. By keeping the first three velocity moments of the equation and ignoring the parallel electric field, these equations give the same Connor-Taylor invariance property¹⁵ as the simple slab equations described in Ref. 14 and Eq. (8) is again a possible solution.

On the other hand, Dupree in a series of papers in the 1960's first proposed the concept of resonance broadening by stating that the wave-particle interaction can be modified by a broadening of the associated resonance denominator $(\omega - \mathbf{k} \cdot \mathbf{v} + i\Delta\omega)^{-1}$ as a result of an incoherent scattering of particle orbits by the waves. This enhanced scattering causes nonlinear saturation of the instability and, in the steady state, also causes anomalous diffusion over the transverse wavelength through¹⁶

$$\Delta\omega \sim k_{\perp}^2 D. \quad (9)$$

This scattering can be considered as an enhanced viscosity (and can exist even only one single unstable mode is present; see, e.g., Ref. 17). Equation (9) can also be viewed as the nonlinear version of Eq. (8) in which the linear drive of ρ_s/L_{Ti} is replaced by its nonlinear counterpart, $\Delta\omega/\Omega_i$.

Let us first compare the results for χ_i in Fig. 1(b) with Eq.(8). Based on the measured mass dependence of $k_r \sim 1/M^{1/4}$ from Fig. 2(a) in the linear stage, the quasilinear χ_i should be independent of mass at saturation. Instead, the simulation χ_i 's give the ratios of (1.35, 1.75, 1.3) for $(H^+/D^+, H^+/T^+, D^+/T^+)$, which seem to have a $1/\sqrt{M}$ dependence. The implication is that either the linear drive or the radial mode structure is

modified. The most likely candidate is the latter, which undergoes drastic breakup during this time. More theoretical understanding is needed. In the steady state, the time-averaged ratios for χ_i are (1.3, 1.8, 1.4) for $(H^+/D^+, H^+/T^+, D^+/T^+)$, which have similar dependence on mass as the quasilinear χ_i 's. Substituting the results from Fig. 2(b) of $k_r \sim 1/\sqrt{M}$ (i.e., $k_r \rho_s \approx \text{const.}$) into Eq. (8), one finds $\chi_i \sim \sqrt{M}$, which gives an opposite scaling. One obvious explanation is that, in the steady state, the linear drive becomes meaningless. One should then use Eq. (9) instead, i.e., replacing the linear drive in Eq. (8) by a nonlinear one. Fig. 4 provides just that and indicates that the fluctuations are less coherent in lighter isotopes, i.e., $\Delta\omega/\Omega_i$'s are larger. One possible reason for this is the radial variation of the temperature gradient for such a plasma. The comparison of $\Delta\omega$ in Fig. 4 can be carried out again by using FWHM. Noting that part of $\Delta\omega$ comes from the FFT sampling error, $2\pi/t_{\text{tot}}$, one can show that $\Delta\omega_H/\Delta\omega_T \approx 5$ and Eq.(8), with the nonlinear drive, gives $\chi_i^H/\chi_i^T \approx 1.7$ which is consistent with the simulation results. The gyrokinetic electrostatic field energy shown in Fig. 1(a) also has the same trend in its dependence on mass as the thermal diffusivity.

In this paper, we have pointed out the origin of favorable isotope scaling in our simulation and demonstrated the inadequacy of the mixing length argument based on the linear drive to predict such a scaling. Moreover, we have presented the first evidence linking resonance broadening and anomalous transport in tokamak plasmas through the 3D toroidal ITG instability. Hopefully, this work helps to underscore the importance of understanding transport phenomena in tokamaks from the first principles of physics.

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Figures

FIG. 1. Time evolution for the ITG instability for the three hydrogenic isotopes in terms of the electrostatic field energy (a) and the ion thermal diffusivity (b).

FIG. 2. The linear radial wavenumber k_r spectra (a) and the time-averaged k_r spectra in the nonlinear steady state (b).

FIG. 3. The time-averaged poloidal k_θ spectra (a) and toroidal k_ϕ spectra (b) in the nonlinear steady state.

FIG. 4. Spatially-averaged frequency spectra along the weak magnetic field side of the midplane for the three hydrogenic isotopes.

Fig. 1

Fig. 2

Fig. 3

Fig. 4

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