**Intrinsic Rotation Driven by Non-Maxwellian Equilibria in Tokamak Plasmas**

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The effect of small deviations from a Maxwellian equilibrium on turbulent momentum transport in tokamak plasmas is considered. These non-Maxwellian features, arising from diamagnetic effects, introduce a strong dependence of the radial flux of cocurrent toroidal angular momentum on collisionality: As the plasma goes from nearly collisionless to weakly collisional, the flux reverses direction from radially inward to outward. This indicates a collisionality-dependent transition from peaked to hollow rotation profiles, consistent with experimental observations of intrinsic rotation.

**Introduction.**—Observational evidence from magnetic confinement fusion experiments indicates that axisymmetric toroidal plasmas (tokamaks) that are initially stationary develop differential toroidal rotation even in the absence of external momentum sources [1–5]. This “intrinsic” rotation can depend sensitively on plasma density and current, and with relatively small variations reversing the rotation direction from co- to countercurrent [3,6–9]. Conservation of angular momentum dictates that the intrinsic rotation is determined by momentum redistribution within the plasma. Since turbulence is the dominant transport mechanism in fusion plasmas [10], one must understand turbulent momentum transport to understand intrinsic rotation.

For the up-down symmetric magnetic equilibria used in most experiments, the turbulent momentum transport for a nonrotating plasma can be shown to be identically zero [11–13] unless one retains formally small effects that are usually neglected. A self-consistent, first-principles theory has been formulated that includes these effects [14,15]. Of these effects, only radial variation of plasma profile gradients [16–19] and slow variation of turbulence fluctuations along the mean magnetic field [20] have been studied, and these studies have not led to a theory that explains the key dependences of intrinsic rotation in the core of tokamaks.

In this Letter we consider the novel effect of small deviations from an equilibrium Maxwellian distribution of particle velocities on turbulent momentum transport. These deviations arise naturally due to diamagnetic effects in plasmas with curved magnetic fields and density and temperature gradients [21]. They vary strongly with quantities such as collisionality, plasma current, and the equilibrium density and temperature gradients in the plasma. We show using direct numerical simulations that these non-Maxwellian features, though small, introduce significant new dependences to the turbulent momentum transport. We discuss the physical origins of the dependences and possible implications for tokamak experiments.

**Momentum transport model.**—Tokamak plasma dynamics typically consist of low amplitude, small scale turbulent fluctuations on top of a slowly evolving macroscopic equilibrium. It is thus natural to employ a mean field theory in which the particle distribution function $f$ is decomposed into equilibrium $F$ and fluctuating $\delta f$ components. The fluctuations are low frequency $\omega$ relative to the ion Larmor frequency $\Omega$ and anisotropic with respect to the equilibrium magnetic field, with characteristic scales of the system size $L$ along the field and the ion Larmor radius $\rho_{i}$ across the field. Expanding $f = f_{0} + f_{1} + \ldots$, employing the smallness parameter $\rho_{s} \equiv \rho / L \sim \omega / \Omega \sim \delta f / F \sim f_{j+1} / f_{j} \ll 1$, and averaging over the fast Larmor motion and over the fluctuation space-time scales, one obtains a coupled set of multiscale gyrokinetic equations for the fluctuation and equilibrium dynamics [22–26].

Typically only the lowest order system of equations for $\delta f$ is considered. However, these equations have been shown to possess a symmetry that prohibits momentum transport in a nonrotating plasma [11–13]. Consequently, we include in our analysis higher order effects arising from corrections to the lowest order (Maxwellian) equilibrium [14,15]. We limit our analysis to these non-Maxwellian corrections because they are known to depend sensitively on plasma collisionality and current, which are key parameters controlling intrinsic rotation in experiments [3,6–9]. We further simplify the analysis by considering only electrostatic fluctuations and by performing the subsidiary expansions $\rho_{s} \ll \nu_{s} \ll 1$ and $\rho_{s} \ll B_{0} / B \ll 1$, where $B$ is the magnitude of the equilibrium magnetic field, $B_{0}$ is the magnitude of the poloidal component, $\nu_{s} \equiv \nu_{q} q R / v_{\|i}$, $v_{\|i}$ is the ion-ion collision frequency, $v_{q} = \sqrt{2T_{i} / m_{i}}$ is the ion thermal speed, $T_{i}$ is the equilibrium ion temperature, $m_{i}$ is the ion mass, $q$ is a measure of the pitch of the magnetic field lines called the safety factor, and $R$ is the major radius of the torus. These are good expansion parameters in typical fusion plasmas.

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**References**


**Figure 1:** Example of intrinsic rotation in a tokamak plasma, showing the direction of the plasma current and the poloidal and toroidal components of the magnetic field. The plasma is initially stationary, but due to small deviations from a Maxwellian equilibrium, a transient intrinsic rotation develops.

**Figure 2:** Simulated turbulent momentum transport in a tokamak plasma, showing the direction of the momentum flux and the poloidal and toroidal components of the magnetic field. The plasma is initially stationary, but due to small deviations from a Maxwellian equilibrium, a transient intrinsic rotation develops.

**Figure 3:** Simulated turbulent momentum transport in a tokamak plasma, showing the direction of the momentum flux and the poloidal and toroidal components of the magnetic field. The plasma is initially stationary, but due to small deviations from a Maxwellian equilibrium, a transient intrinsic rotation develops.

**Figure 4:** Simulated turbulent momentum transport in a tokamak plasma, showing the direction of the momentum flux and the poloidal and toroidal components of the magnetic field. The plasma is initially stationary, but due to small deviations from a Maxwellian equilibrium, a transient intrinsic rotation develops.
Our analysis is done in the frame rotating toroidally with the $E \times B$ rotation frequency $\omega_{\perp,E} = -(c/R_B p) (\partial \Phi_0 / \partial r)$, with $c$ the speed of light, $\Phi_0$ the lowest order equilibrium electrostatic potential, and $r$ a radial coordinate labeling surfaces of constant magnetic flux. Using $(R, e, \mu)$ variables, with $R$ the position of the center of a particle’s Larmor motion, $e = m u^2 / 2$ the particle’s kinetic energy, $\mu = m v_r^2 / 2B$ the particle’s magnetic moment, $v$ the particle’s speed in the rotating frame, and $\perp$ indicating the component perpendicular to the magnetic field, the resulting equation for the fluctuation dynamics is

$$\frac{D g_s}{D t} + (\mathbf{v} \cdot \nabla) + v_{Ds} \cdot \nabla \perp \left( g_s - Z_s e (\varphi) \frac{\partial \mathbf{F}_s}{\partial \varphi} \right) + \langle \delta v_E \rangle \cdot \left( \nabla \perp g_s + \mathbf{v}_s \times \mathbf{R} \right) = Z_s e v_{\parallel} \frac{\partial g_s}{\partial \varphi} + \langle C_s \rangle,$$

where $g = \delta f_1 + \delta f_2$, $\mathbf{v}$ is particle velocity, the subscript \parallel denotes the component along the equilibrium magnetic field, $Z e$ is particle charge, $\varphi = \delta \phi_1 + \delta \phi_2$ is the fluctuating electrostatic potential, $\mathbf{F}_0 = 0 + \Phi_0 + \Phi_1$ is the equilibrium electrostatic potential, $\mathbf{F} = F_0 + F_1$, $D/ Dt = \partial / \partial t + \mathbf{v} \cdot \nabla$ is an average along Larmor angle at fixed $R$, $\mathbf{v}_{Ds} = \mathbf{v}_{Ms} + \mathbf{v}_{Cs}$, with $\mathbf{v}_{Cs}$ the drift velocity due to the Coriolis effect and $\mathbf{v}_{Ms}$ the drift velocity due to curvature and inhomogeneity in the equilibrium magnetic field, $\delta v_E = (c/B) \mathbf{b} \times \nabla \perp \varphi$ and $\mathbf{v}_E = (c/B) \mathbf{b} \times \nabla \mathbf{F}$ are $E \times B$ drift velocities, $\mathbf{b}$ is the unit vector along the magnetic field, $B_{\perp}$ is the toroidal component of the magnetic field. The subscript $s$ denotes species, and $C_s$ describes the effect of Coulomb collisions on species $s$.

Tokamak plasmas are sufficiently collisional that the distribution of particle velocities is close to Maxwellian; i.e., $f_0 = F_0 = F_M$, with $F_M$ a Maxwellian. Equilibrium deviations from $F_M$ are determined by the kinetic equation [21],

$$\mathbf{v}_{\parallel} \cdot \nabla H_{1s} + \mathbf{v}_{Ms} \cdot \nabla F_{Ms} = C_s [H_{1s}],$$

where $H_1 = F_1 + Z e \Phi_1 F_M / T$. Finally, the electrostatic potentials are obtained and the system closed by enforcing quasineutrality:

$$\sum_s Z_s \int d^3 \mathbf{v} \left( g_s + \frac{Z_s e}{T_s} \langle (\varphi) - \varphi \rangle F_{Ms} \right) = 0,$$  \hspace{1cm} (3)

$$\sum_s Z_s \int d^3 \mathbf{v} \left( H_{1s} - \frac{Z_s e}{T_s} \Phi_1 F_{Ms} \right) = 0.$$  \hspace{1cm} (4)

With $g_s$ and $\varphi$ determined by Eqs. (1)–(4), the turbulent radial fluxes of energy $Q$ and toroidal angular momentum $\Pi$ are given by

$$Q_s = \langle e_s \delta f_1 \delta \mathbf{v}_E \cdot \nabla r \rangle_{\lambda},$$  \hspace{1cm} (5)

$$\Pi = \sum_s \langle m_s R^2 \delta f_1 (\mathbf{v} \cdot \nabla \xi) \delta \mathbf{v}_E \cdot \nabla r \rangle_{\lambda},$$  \hspace{1cm} (6)

where $f = g + Ze (\varphi - \varphi) F_M / T$, $\xi$ is the toroidal angle, $\mathbf{v} = \mathbf{v} + R^2 \omega_{\perp,E} \mathbf{F}$ is the particle velocity in the nonrotating frame, and $\langle a \rangle_{\lambda} = \int dt \int d^3 r \int d^3 \mathbf{v} a / \int dt \int d^3 r$ is an integral over all velocity space, over the volume between two surfaces of constant $r$ separated by a distance $w$ ($\rho \ll w \ll L$, and over a time interval $\Delta t$ ($R_0 / v_T \ll \Delta t \ll \rho_s$). This combined phase space and time average is assumed to encompass several turbulence correlation lengths and times.

**Results and analysis.**—We obtain the correction $F_1$ to the equilibrium Maxwellian and the corresponding electrostatic potential $\Phi_1$ by solving Eqs. (2) and (4) using the drift kinetic code NEO [27]. These quantities are then input to the $\delta f$ gyrokinekinetic code G$S$2 [28], which we have modified to solve Eqs. (1) and (3) in the presence of $F_1$ and $\Phi_1$. To calculate the “intrinsic” momentum flux that is present even for a nonrotating plasma, we set the total toroidal angular momentum in a constant-flux surface, which consists of diamagnetic and $E \times B$ contributions, to zero: $\sum_s \langle m_s R^2 (\mathbf{v} \cdot \nabla \xi) F_1 \rangle / \sum_s \langle m_s R^2 \rangle$ the diamagnetic contribution to the toroidal rotation frequency and $n$ the number density. The nonzero $E \times B$ rotation needed to cancel the diamagnetic rotation breaks the symmetry of the lowest order gyrokinetic equation and thus contributes to momentum transport, as do the non-Maxwellian equilibrium corrections we have included.

We consider a simple magnetic equilibrium with concentric circular flux surfaces known as the cyclone base case [29], which has been benchmarked extensively in the fusion community. The equilibrium is fully specified by the Miller model [30], with $q = 1.4$, $\delta = \partial \ln q / \partial \ln r = 0.8$, $e = r / R_0 = 0.18$, $R_0 / L_n = 2.2$, and $R_0 / L_T = 6.9$, where $r$ is the minor radius at the constant-flux surface of interest, $R_0$ is the major radius evaluated at $r = 0$, and $L_n$ and $L_T$ are the density and temperature gradient scale lengths for both ions and electrons. In order to obtain the gradient of $F_1$ appearing in Eq. (1), we must additionally specify the radial dependence of $L_n$ and $L_T$, which we take to be constant in $r$ ($\partial L_T / \partial r = \partial L_n / \partial r = 0$) for our base case.

With these base case parameters specified, we conduct a series of simulations with kinetic electrons and deuterium ions, varying $v_s$ and $\kappa = R_0^2 \partial^2 / \partial \ln q / \partial \ln r^2$ about the baseline value of $v_s = 0.003$, $\kappa = 0$. Our G$S$2 simulations use 32 grid points in the coordinate parallel to the magnetic field (the poloidal angle), 12 grid points in $e$, 37 grid points in $\lambda = \mu / e$, and 128 and 22 Fourier modes in the radial and binormal coordinates, respectively. The box size in both the radial and binormal coordinates is approximately $125 \rho_i$.

The resulting $\Pi / Q_s$ values as a function of $v_s$ are shown in Fig. 1. We normalize $\Pi$ by $Q_s$, which is always positive, to remove any dependence of overall turbulence amplitude...
on collisionality. Note that $F_1$, and thus $\omega_{\xi,E} = -\omega_{\xi,d}$, varies with collisionality, as indicated in Table I. For nearly collisionless plasmas, $\Pi/Q_i$ is negative, indicating a radially inward flux of cocurrent angular momentum that would contribute to a centrally peaked rotation profile. The ratio $\Pi/Q_i$ increases with $\nu_*$, passing through zero and becoming positive when $\nu_* \sim \epsilon^{3/2}$. For $\nu_* \geq \epsilon^{3/2}$, the radially outward flux of cocurrent angular momentum would contribute to a hollow rotation profile.

In Fig. 2, we show results from a series of simulations in which we independently set the $E \times B$ rotation (including its derivative) and the diamagnetic effects, represented by $F_1$, to zero. These are given by the blue and red curves, respectively. We see that the $E \times B$ rotation causes an inward momentum flux, with $\Pi/Q_i$ increasing in magnitude with $\nu_*$. The non-Maxwellian correction $F_1$ gives a $\Pi/Q_i$ that goes from slightly negative to large and positive as $\nu_*$ is increased. A partial cancellation between these effects gives the actual $\Pi/Q_i$.

To explore in more detail the origin of the sign reversal of $\Pi/Q_i$, it is convenient to express the ion energy flux in the diffusive form $Q_i = -n_i \chi_i \partial T_i/\partial r$, and to decompose the momentum flux as

$$\Pi = -mnR_0^2 \left( \frac{\partial \omega_{\xi,d}}{\partial r} \chi_{\phi,d} + \frac{\partial \omega_{\xi,E}}{\partial r} \chi_{\phi,E} \right)$$

$$- mnR_0^2 (\omega_{\xi,d} P_d + \omega_{\xi,E} P_E) + \Pi_{\text{other}}, \quad (7)$$

where $\chi_{\phi,d}$ and $P_d$ are diffusion and “pinch” coefficients, respectively, for the diamagnetic rotation, and $\chi_{\phi,E}$ and $P_E$ play the same roles for the $E \times B$ rotation. Equation (8) can be viewed as a Taylor expansion of $\Pi$ for small values of the rotation and rotation shear. The quantity $\Pi_{\text{other}}$ accounts for all other sources of $\Pi$ that arise due to $F_1[\omega_{\xi,d}(r) = \omega_{\xi,E}(r) = 0]$; e.g., the equilibrium parallel heat flow and other higher order velocity moments of $F_1$ will contribute to $\Pi_{\text{other}}$. Using the fact that $\omega_{\xi,E} = -\omega_{\xi,d}$ for a nonrotating plasma, we have

$$\Pi = -mnR_0^2 \left( \frac{\partial \omega_{\xi,d}}{\partial r} \chi_{\phi,\text{eff}} + \omega_{\xi,E} P_{\text{eff}} \right) + \Pi_{\text{other}}, \quad (8)$$

where $\chi_{\phi,\text{eff}} = \chi_{\phi,d} - \chi_{\phi,E}$ and $P_{\text{eff}} = P_d - P_E$.

Changing $\nu_*$ can alter $\Pi/Q_i$ in multiple ways. First, the effective turbulent pinch and diffusion coefficients, $P_{\text{eff}}/\chi_i$ and $\chi_{\phi,\text{eff}}/\chi_i$, can be modified either directly by collisions or indirectly by the $\nu_*$-dependent rotation and rotation gradient. By independently varying $\nu_*$, $\omega_{\xi,E}$, and $\partial \omega_{\xi,d}/\partial r$ in GS2 turbulence simulations with fixed $F_1$ and $\Phi_\rho$, we found that such modifications of the pinch and diffusion coefficients were minor. Furthermore, the turbulence type, characterized by the dominant linear instability mechanism, remained the same (ion-temperature-gradient driven) for all simulations.

With $\chi_{\phi,\text{eff}}/\chi_i$ and $P_{\text{eff}}/\chi_i$ approximately independent of $\nu_*$, we see from Eq. (8) that the $\nu_*$ dependence of $(\Pi - \Pi_{\text{other}})/Q_i$ comes entirely from the change of $\omega_{\xi,d}$ and $\partial \omega_{\xi,d}/\partial r$ with $\nu_*$, given in Table I. In order to calculate $(\Pi - \Pi_{\text{other}})/Q_i$, we ran a series of simulations in which we used a modified $F_1$ that was constrained to produce pure rotation so that $\Pi_{\text{other}} = 0$. The results are shown in Fig. 2. We see that $(\Pi - \Pi_{\text{other}})/Q_i$ is always positive and increases approximately linearly with $\partial \omega_{\xi,d}/\partial r$, as diffusion was found to dominate over pinch in these cases. This indicates that equal and opposite diamagnetic and $E \times B$ rotations do not lead to a complete cancellation of momentum transport [31]. The increase in $(\Pi - \Pi_{\text{other}})/Q_i$ with $\nu_*$ accounts for just over half of the total increase in

![FIG. 1](color online). Ratio of radial fluxes of ion toroidal angular momentum $\Pi$ and energy $Q_i$ vs normalized ion-ion collision frequency $\nu_*$.

![FIG. 2](color online). Ratio of radial fluxes of ion toroidal angular momentum $\Pi$ and energy $Q_i$ vs normalized ion-ion collision frequency $\nu_*$ for: the base simulations (solid black line), simulations with no $E \times B$ rotation to balance the diamagnetic rotation (short dashed blue line), simulations with no correction $F_1$ to the Maxwellian equilibrium (long dashed red line), and simulations with $\Pi_{\text{other}} = 0$ (dotted green line).

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**TABLE I.** Collisionality dependence of $\omega_{\xi,d}$.

<table>
<thead>
<tr>
<th>$\nu_*$</th>
<th>$k_0 \omega_{\xi,d}$</th>
<th>$k_1 \omega_{\xi,d}$</th>
<th>$k_2 \omega_{\xi,d}$</th>
<th>$k_3 \omega_{\xi,d}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.003</td>
<td>0.030</td>
<td>0.059</td>
<td>0.089</td>
<td>0.148</td>
</tr>
<tr>
<td>0.091</td>
<td>0.114</td>
<td>0.127</td>
<td>0.137</td>
<td>0.153</td>
</tr>
<tr>
<td>-0.447</td>
<td>-0.577</td>
<td>-0.651</td>
<td>-0.701</td>
<td>-0.776</td>
</tr>
<tr>
<td>-0.829</td>
<td>-0.891</td>
<td>-0.981</td>
<td>-1.057</td>
<td>-1.133</td>
</tr>
</tbody>
</table>
TABLE II. Temperature profile dependence of $\omega_{c,d}$.  

<table>
<thead>
<tr>
<th>$-L_T^2 \frac{\partial^2 \ln T}{\partial r^2}$</th>
<th>-1</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\frac{\partial \omega_{c,d}}{\partial r}$</td>
<td>-1.116</td>
<td>-0.447</td>
<td>-0.105</td>
<td>0.223</td>
<td>0.835</td>
</tr>
</tbody>
</table>

$\Pi / Q_i$ over the range of $\nu_*$ we have considered. The rest of the increase, as well as the negative offset needed to give the sign reversal in $\Pi / Q_i$ must come from $\Pi_{therm} / Q_i$.

To see how these results may be modified for different plasma profiles, we also conducted a series of simulations in which we fixed $\nu_*=0.003$ and varied $\kappa = R_0^2 \partial^2 \ln T / \partial r^2$. Since the calculation of $F_1$ in NEQ depends on $R_0 / L_T$, varying $\kappa$ affects $\partial F_1 / \partial r$ but not $F_1$ itself. Consequently, $\partial \omega_{c,d} / \partial r$ varies with $\kappa$ (see Table II) while $\omega_{c,d}$ itself remains fixed. The change in $\Pi / Q_i$ with $\kappa$ is shown in Fig. 3. As was the case in the $\nu_*$ study, the $E \times B$ and $F_1$ contributions to $\Pi / Q_i$ partially cancel, though in this case each contribution independently changes sign with $\kappa$. The net result is a relatively weak variation of $\Pi / Q_i$ with no sign reversal.

Discussion.—The sign reversal of $\Pi / Q_i$ shown in Fig. 1 suggests a transition from peaked to hollow rotation profiles when $\nu_* \sim \epsilon^{3/2}$. This is consistent with experimental results, which show such transitions at similar $\nu_*$ values when density (proportional to $\nu_*$) is increased or current (inversely proportional to $\nu_*$) is decreased [3,6,9,32]. Furthermore, our observation that the normalized turbulence diffusion and pinch coefficients vary only minimally during the transition agree with recent experimental observations showing that the fundamental turbulence characteristics are unaltered as the rotation reverses direction [9].

From Fig. 2 and the analysis following Eq. (8), it is evident that a combination of effects leads to the sign reversal of $\Pi / Q_i$. However, the sign reversal fundamentally originates from the $\nu_*$ dependence of $F_1$, which has been extensively studied and is the main concern of “neoclassical” theory (see, e.g., [21,33]). For $\nu_* \ll \epsilon^{3/2}$, known as the “banana” regime, all particle orbits are collisionless. However, for $\epsilon^{3/2} \ll \nu_* \ll 1$, known as the “plateau” regime, low energy particles that are trapped in the equilibrium magnetic well become collisional. For a plasma perfectly in the banana or plateau regimes, one can show that $F_1$, and thus our $\Pi / Q_i$, becomes independent of $\nu_* [21,33]$. It is only when transitioning between these regimes that $\Pi / Q_i$ varies with $\nu_*$. So, while different profiles of quantities such as density, temperature, and current may alter or eliminate the transitions with $\nu_*$ discussed above, transitions can only occur for $\nu_* \sim \epsilon^{3/2}$.

During the transition between collisionality regimes, the equilibrium poloidal flow obtained from neoclassical theory reverses direction. If the diamagnetic effects discussed here are responsible for the reversal of the toroidal rotation, an experimental signature would thus be a correlation between the reversal of the toroidal and poloidal flows [34].

Finally, we reiterate that in our analysis we retained small terms (namely the diamagnetic effects that give rise to departures from a Maxwellian equilibrium distribution) in the multiscale gyrokinetic expansion, while we neglected other terms (radial profile variation, certain effects arising from the slow variation of fluctuations along the magnetic field, etc.) that may be of the same size. There are two justifications for this. First, if the fluctuation amplitudes and scales do not vary strongly with $B_0 / B$, then the diamagnetic effects considered here dominate so that our model is fully self-consistent [14,15]. Second, the small effects we have neglected are not expected to have a particularly strong dependence on collisionality. Thus, while inclusion of these effects may provide an offset to the momentum transport, we do not expect them to modify the variation of $\Pi / Q_i$ with $\nu_*$ presented here.

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[26] I. G. Abel et al. (to be published).
[34] M. Reinke (private communication).