Drift-Kinetic Simulations of Neoclassical Transport

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GENERAL ATOMICS

Motivation for the NEO code

- **Develop a practical tool for high-accuracy neoclassical calculations, which includes:**
  - Self-consistent coupled ion-electron physics
  - Multiple ion species
  - Poloidal correction to the potential
  - General geometry
  - Rotation effects

- **Provide a stepping-stone toward a full-F Gyrokinetic + Neoclassical solver**
  - Serve as a framework to explore new formulations which will allow calculation of the neoclassical E_r^0
  - Provide a tool for use in steady-state gyrokinetic transport simulations: TGYRO → coupled GYRO + NEO simulations

Hierarchy of Equations

Based on expansion of the DKP eqns in powers of ρ_{*i}

$O(1)$:

$$v_\parallel \hat{b}\cdot\nabla f_{0a} - \frac{Z_a e}{m_a} v_\parallel \hat{b}\cdot\nabla\Phi_0 \frac{\partial f_{0a}}{\partial\varepsilon} - C_{aa}\left(f_{0a}, f_{0a}\right) = 0$$

$$\sum_a Z_a e n_{0a} = 0$$

Not solved

$$f_{0a} = F_{Ma}$$

$O(\rho_{*i})$:

$$v_\parallel \hat{b}\cdot\nabla f_{1a} - \frac{Z_a e}{m_a} v_\parallel \hat{b}\cdot\nabla\Phi_1 \frac{\partial f_{0a}}{\partial\varepsilon} - \sum_b C_{ab}^L\left(f_{1a}, f_{1b}\right) = -\vec{v}_D\cdot\nabla f_{0a} + \frac{Z_a e}{m_a}\vec{v}_D\cdot\nabla\Phi_0\frac{\partial f_{0a}}{\partial\varepsilon}$$

$$0 = \sum_a Z_a e \int d^3v f_{1a}$$

Standard neoclassical

$$\Gamma_{2a} = \left\langle \int d^3v\left(f_{0a}\vec{v}_E^{(1)}\cdot\nabla r + f_{1a}\vec{v}_D\cdot\nabla r\right)\right\rangle$$

$$Q_{2a} = \left\langle \int d^3v m_a\varepsilon\left(f_{0a}\vec{v}_E^{(1)}\cdot\nabla r + f_{1a}\vec{v}_D\cdot\nabla r\right)\right\rangle$$

$O(\rho_{*i}^2)$:

$$v_\parallel \hat{b}\cdot\nabla f_{2a} - \frac{Z_a e}{m_a} v_\parallel \hat{b}\cdot\nabla\Phi_2 \frac{\partial f_{0a}}{\partial\varepsilon} - \sum_b C_{ab}^L\left(f_{2a}, f_{2b}\right) = -\vec{v}_D\cdot\nabla f_{1a} + \frac{Z_a e}{m_a}\vec{v}_D\cdot\nabla\Phi_1\frac{\partial f_{0a}}{\partial\varepsilon} + \vec{v}_E^{(0)}\cdot\nabla f_{1a} + \vec{v}_E^{(1)}\cdot\nabla f_{0a}$$
$$+\frac{Z_a e}{m_a}\left(v_\parallel\hat{b}\cdot\nabla\Phi_1 + \vec{v}_D\cdot\nabla\Phi_0\right)\frac{\partial f_{1a}}{\partial\varepsilon} + \dot{\mu}\frac{\partial f_{1a}}{\partial\mu} + S_{2a}{}^{*}$$

$$-\sum_a \frac{n_{0a}Z_s^2 e^2}{T_{0a}}\rho_a^2\left|\nabla r\right|^2\frac{\partial^2\Phi_0}{\partial r^2} = \sum_a Z_a e\int d^3v f_{2a}$$

* required for solvability

FOW correction

$$\Gamma_{3a} = \left\langle \int d^3v\left(f_{0a}\vec{v}_E^{(2)}\cdot\nabla r + f_{2a}\vec{v}_D\cdot\nabla r + f_{1a}\vec{v}_E^{(1)}\cdot\nabla r\right)\right\rangle$$

$$Q_{3a} = \left\langle \int d^3v m_a\varepsilon\left(f_{0a}\vec{v}_E^{(2)}\cdot\nabla r + f_{2a}\vec{v}_D\cdot\nabla r + f_{1a}\vec{v}_E^{(1)}\cdot\nabla r\right)\right\rangle$$

Basic Properties I: The Poisson Equation

At a given order, the Poisson eqn and the DKE are uncoupled

The kth-order Poisson eqn is not needed to determine the kth-order fluxes:

$$f_{ka} = g_{ka} - f_{0a}\frac{Z_a e}{T_{0a}}\Phi_k$$

$$\Downarrow$$

$$O(\rho_{*i}): \quad \sum_b D_{ab}(g_{1a}, g_{1b}) = R_{1a}(f_{0a}, \Phi_0) \qquad \rightarrow \Gamma_{2a} = \left\langle \int d^3v\, g_{1a}(\vec{v}_D \cdot \nabla r) \right\rangle$$

$$\sum_a \frac{n_{0a} Z_a^2 e^2}{T_{0a}} \Phi_1 = \sum_a Z_a e \int d^3v\, g_{1a}$$

$$O(\rho_{*i}^2): \quad \sum_b D_{ab}(g_{2a}, g_{2b}) = R_{2a}(f_{0a}, g_{1a}, \Phi_0, \Phi_1) + S_{2a} \qquad \rightarrow \Gamma_{3a} = \left\langle \int d^3v \left(g_{2a}\vec{v}_D \cdot \nabla r + f_{1a}\vec{v}_E^{(1)} \cdot \nabla r \right) \right\rangle$$

$$\sum_a \frac{n_{0a} Z_a^2 e^2}{T_{0a}} \left(\Phi_2 - \rho_a^2 \frac{\partial^2 \Phi_0}{\partial r^2} \right) = \sum_a Z_a e \int d^3v\, g_{2a} \qquad \left(S_{2a}(\varepsilon) = -\frac{1}{2}\int_{-1}^{1} d\xi \langle R_{2a} \rangle \right)$$

Not true for the time-dependent problem: $\frac{\partial f_{ka}}{\partial t} \rightarrow \frac{\partial g_{ka}}{\partial t} - f_{0a}\frac{Z_a e}{T_{0a}}\frac{\partial \Phi_k}{\partial t}$

Basic Properties II: Ambipolarity Property

Requires complete cross-species collisional coupling

Operate on the kinetic equation with $\langle \int d^3v (v_{\|}/B) \ldots \rangle$:

$$\Gamma_{2a} = -\left\langle \frac{I}{\psi'\Omega_a} \int d^3v \, v_{\|} \sum_b C_{ab} g_{1b} \right\rangle$$

$$\Downarrow$$

$$\sum_a Z_a \Gamma_{2a} = -c \left\langle \frac{I}{\psi' e B} \int d^3v \sum_{a,b} m_a v_{\|} C_{ab} g_{1b} \right\rangle$$

$I(\psi) = RB_t$

ψ : poloidal flux / (2π)

$\frac{I}{\psi'} \rightarrow \frac{qR_0}{r}$ (s - α geometry)

The plasma maintains ambipolarity only if the momentum conservation properties of C_{ab} are properly maintained.

Model forms of the linearized collision operator

- Connor Model

$$C_{ab}^{L} = \nu_{ab} L f_{1a} + P_1\left(\mathrm{v}_{\|}/\mathrm{v}\right)\left(\nu_{ab}\mathrm{v}\frac{r_{ba}}{\mathrm{v}_{ta}^{2}}\right) f_{0a}$$

- Zeroth Order Hirshman-Sigmar Operator

$$C_{ab}^{L} = \nu_{ab}^{D} L f_{1a} + P_1\left(\mathrm{v}_{\|}/\mathrm{v}\right)\left[\nu_{ab}^{s}\mathrm{v}\frac{r_{ba}}{\mathrm{v}_{ta}^{2}} + \left(\nu_{ab}^{D} - \nu_{ab}^{s}\right)\frac{u_{a1}(\mathrm{v})}{\mathrm{v}}\right] f_{0a}$$

- Full Hirshman-Sigmar Operator

$$C_{ab}^{L} = \nu_{ab}^{D} L f_{1a} + P_1\left(\mathrm{v}_{\|}/\mathrm{v}\right)\left[\nu_{ab}^{s}\mathrm{v}\frac{r_{ba}}{\mathrm{v}_{ta}^{2}} + \left(\nu_{ab}^{D} - \nu_{ab}^{s}\right)\frac{u_{a1}(\mathrm{v})}{\mathrm{v}} + \left(\nu_{ab}^{h} h_{ba} + \nu_{ab}^{k} k_{ab}\right)\frac{\mathrm{v}^{3}}{\mathrm{v}_{ta}^{4}}\right] f_{0a}$$

$$+ \frac{1}{\mathrm{v}^{2}}\frac{\partial}{\partial \mathrm{v}}\left[\frac{1}{2}\nu_{\mathrm{ab}}^{\|}\mathrm{v}^{4}\left(\frac{\partial n_{1a}}{\partial \mathrm{v}} - \frac{\mathrm{v}}{\mathrm{v}_{\mathrm{ta}}^{2}} q_{ba}\right) f_{0a}\right] + P_2\left(\mathrm{v}_{\|}/\mathrm{v}\right)\left[\nu_{ab}^{p}\mathrm{v}^{2}\frac{5\pi_{ba}}{4\mathrm{v}_{ta}^{4}} - \nu_{ab}^{E}\frac{\pi_{1a}(\mathrm{v})}{\mathrm{v}^{2}}\right] f_{0a}$$

Connor, PP 15, 765 (1973); Hirshman & Sigmar, NF 21, 1079 (1981).

The NEO Code

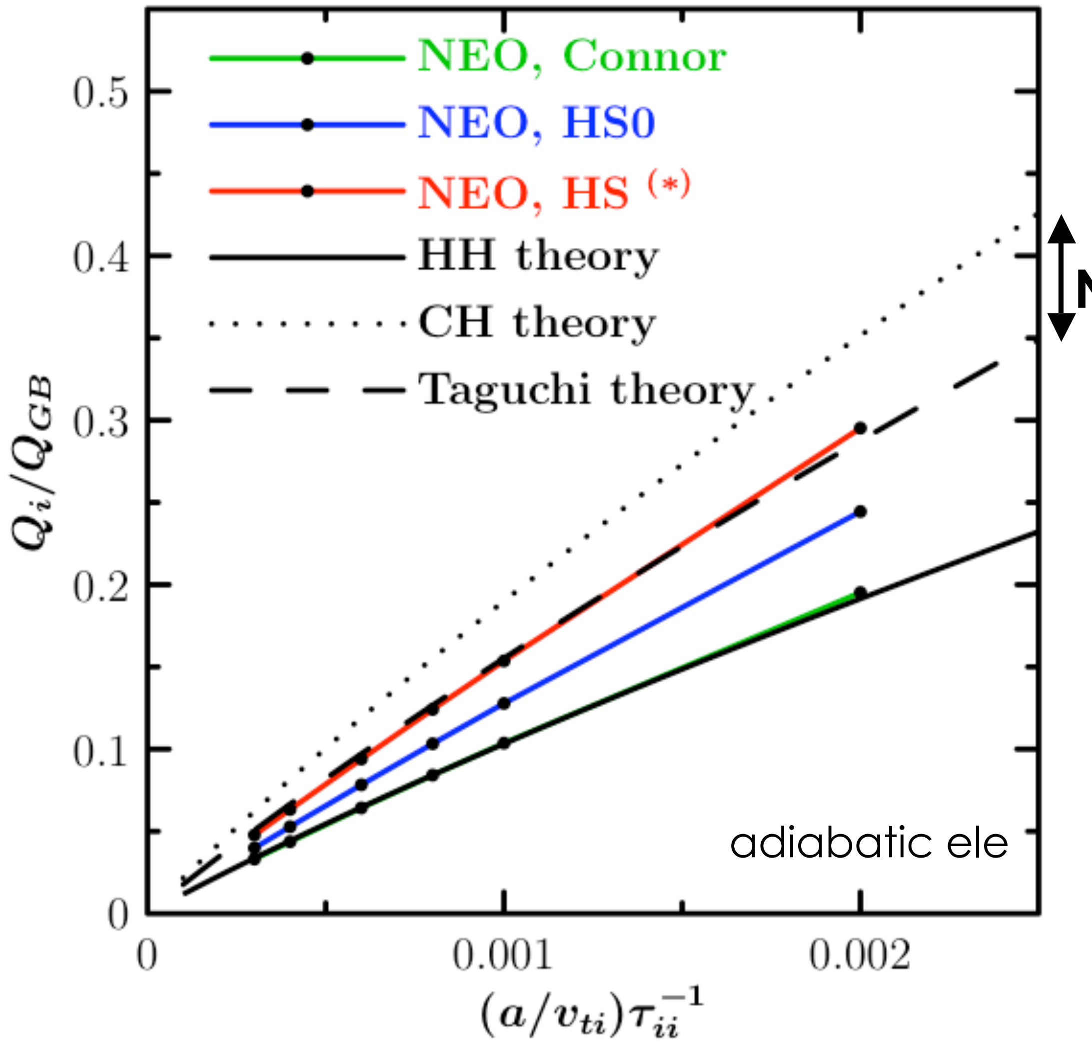
$$g_{ka}(r,\theta,\xi,\varepsilon) = f_{0a}(r,\varepsilon)\sum_{m=0}^{N_\xi -1}\sum_{n=0}^{N_\varepsilon -1} P_m(\xi)T_n(z)c^{a}_{m,n}(r,\theta)$$

- **Mesh in $\{r_i,\theta_j\}$**
- **Legendre polynomials in $\xi=v_{||}/v$**
  - collocation integrals done exactly
- **Chebyshev polynomials in $\varepsilon=v^2/2$**
  ($z=2(\varepsilon/\varepsilon_{max})^{1/2}-1$, typically $\varepsilon_{max}=16v_{ta}^2$)
  - collocation integrals done with composite higher-order Gauss-Legendre quadrature
    - collision integrals, which are multi-scale, can be done to high accuracy (8-10 significant digits)

⇒ **Sparse matrix system:** $A^{aa',jj'}_{mm',nn'}c^{a',j'}_{m',n'} = b^{a,j}_{m,n}$

Verification of NEO

Comparison with analytical theories in the banana regime



Only the full HS op recovers Taguchi's theory.

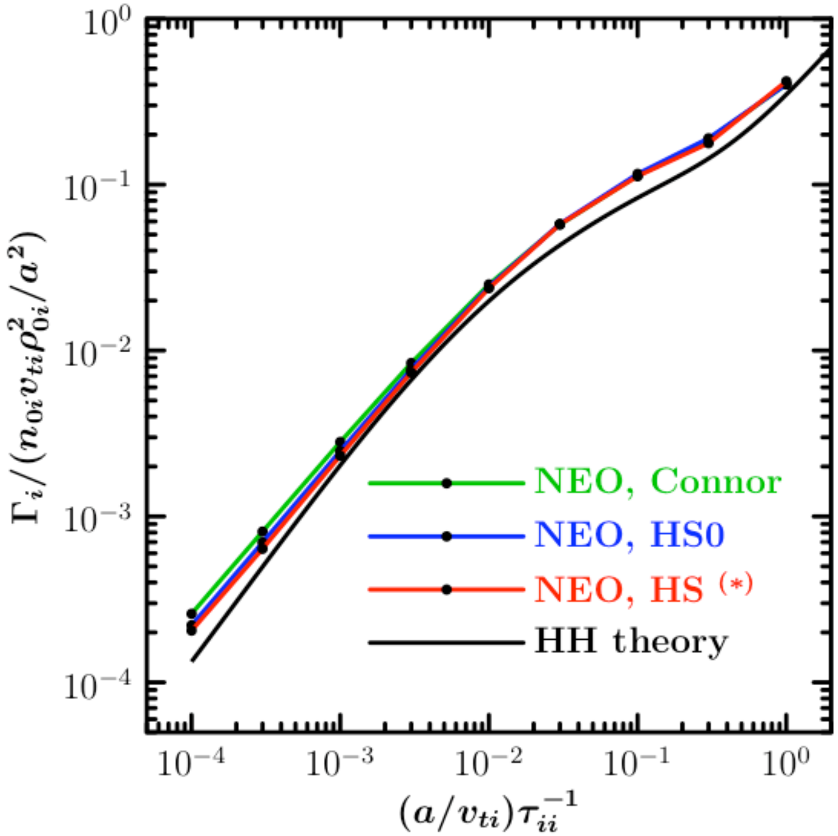
Note: **Chang-Hinton theory overestimates Q_i.**

GA standard parameters:
(s-α geometry)
$R_0/a=3$ $a/L_n=1$
$r/a=0.5$ $a/L_T=3$
$q=2$ $T_{0i}=T_{0e}$

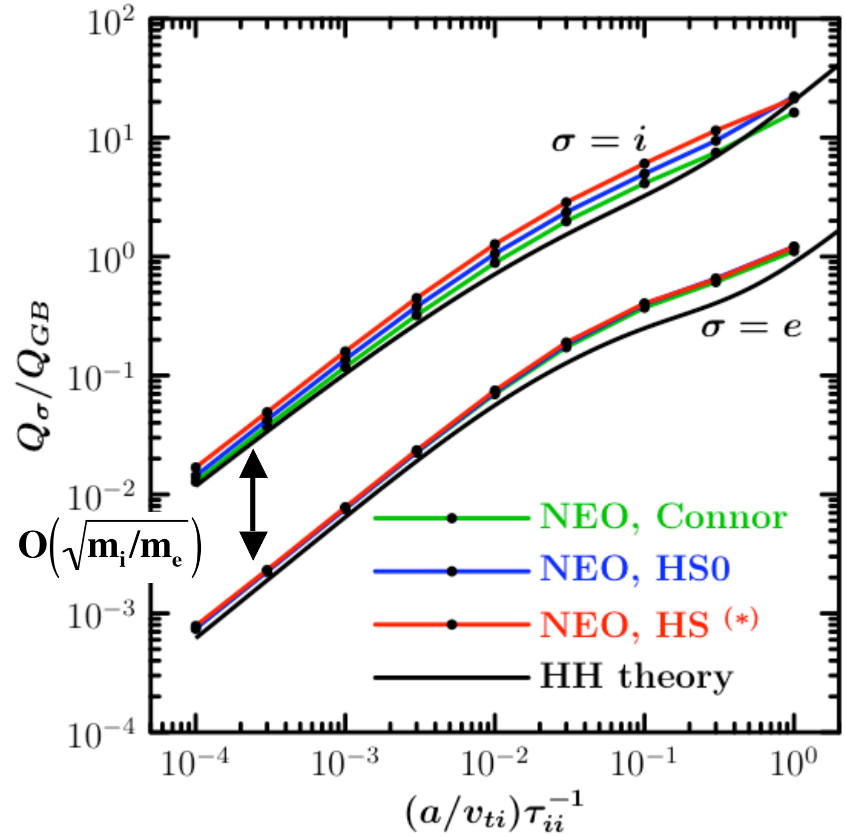
Hinton & Hazeltine, RMP 48, 239 (1976).
Chang & Hinton, PF 25, 1493 (1982).
Taguchi, PPCF 30, 1897 (1988).

Results with self-consistent electron dynamics
Comparison of 2nd order fluxes with analytical theory

Ambipolarity has been confirmed.



Connor coll op & HS0 coll op consistently underestimate Q.



Full electron-deuterium mass ratio used.

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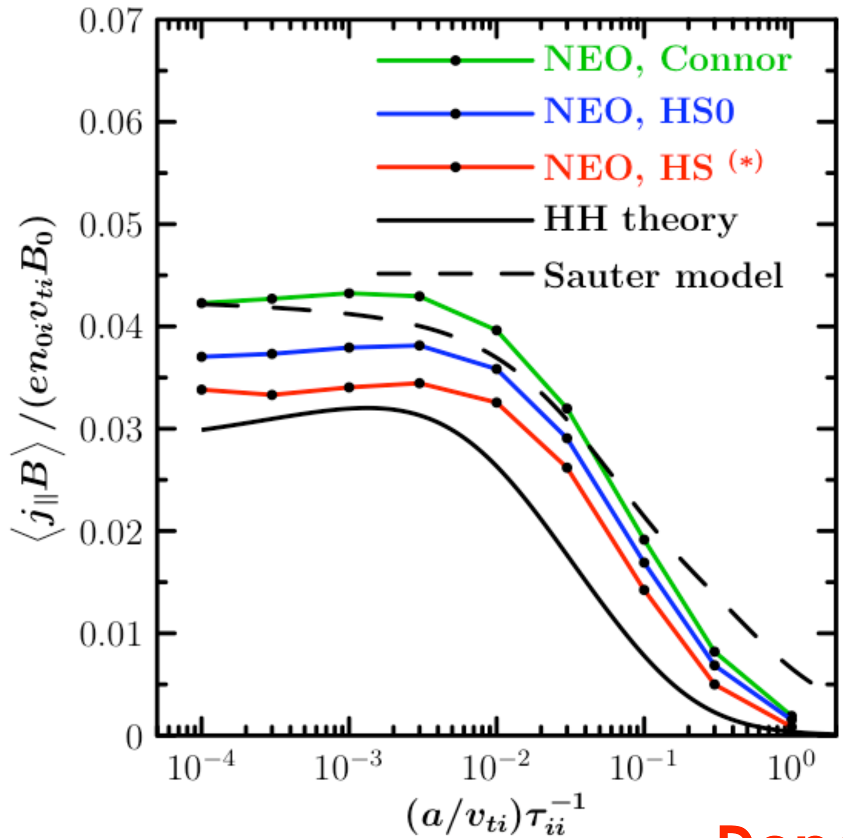
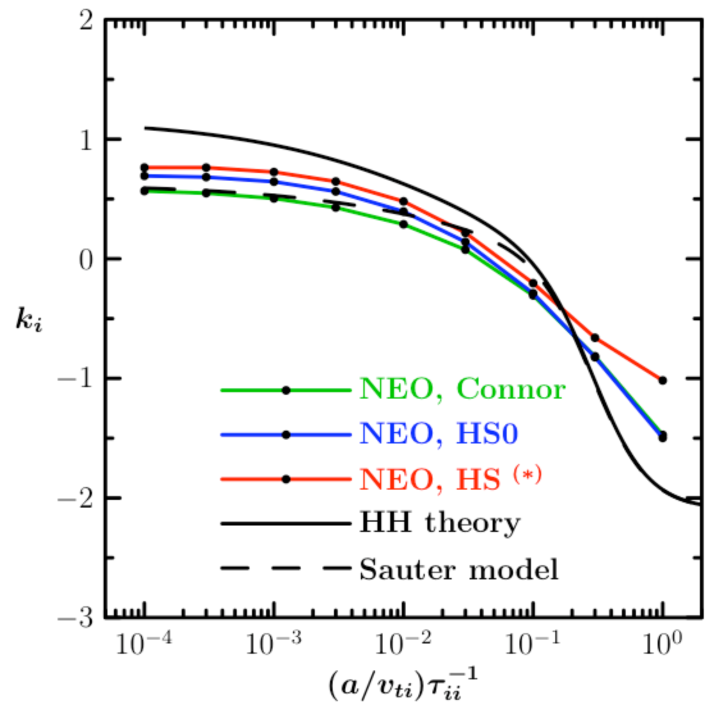
Results with self-consistent electron dynamics

Comparison of 1st order parallel flows with analytical theory



Standard neoclassical relation:

$$\langle u_\parallel B\rangle_i = \frac{cT_{0i}}{Z_i e}\frac{I}{\psi'}\left(-\frac{Z_i e}{T_{0i}}\frac{\partial \Phi_0}{\partial r} + \frac{1}{L_{ni}} + (1-k_i)\frac{1}{L_{Ti}}\right)$$



Hinton & Hazeltine, RMP 48, 239 (1976).

Sauter et al, PoP 6, 2834 (1999); PoP 9, 5140 (2002).

Dependence of k_i on ε & ν_{*i} is coupled and difficult to predict analytically.

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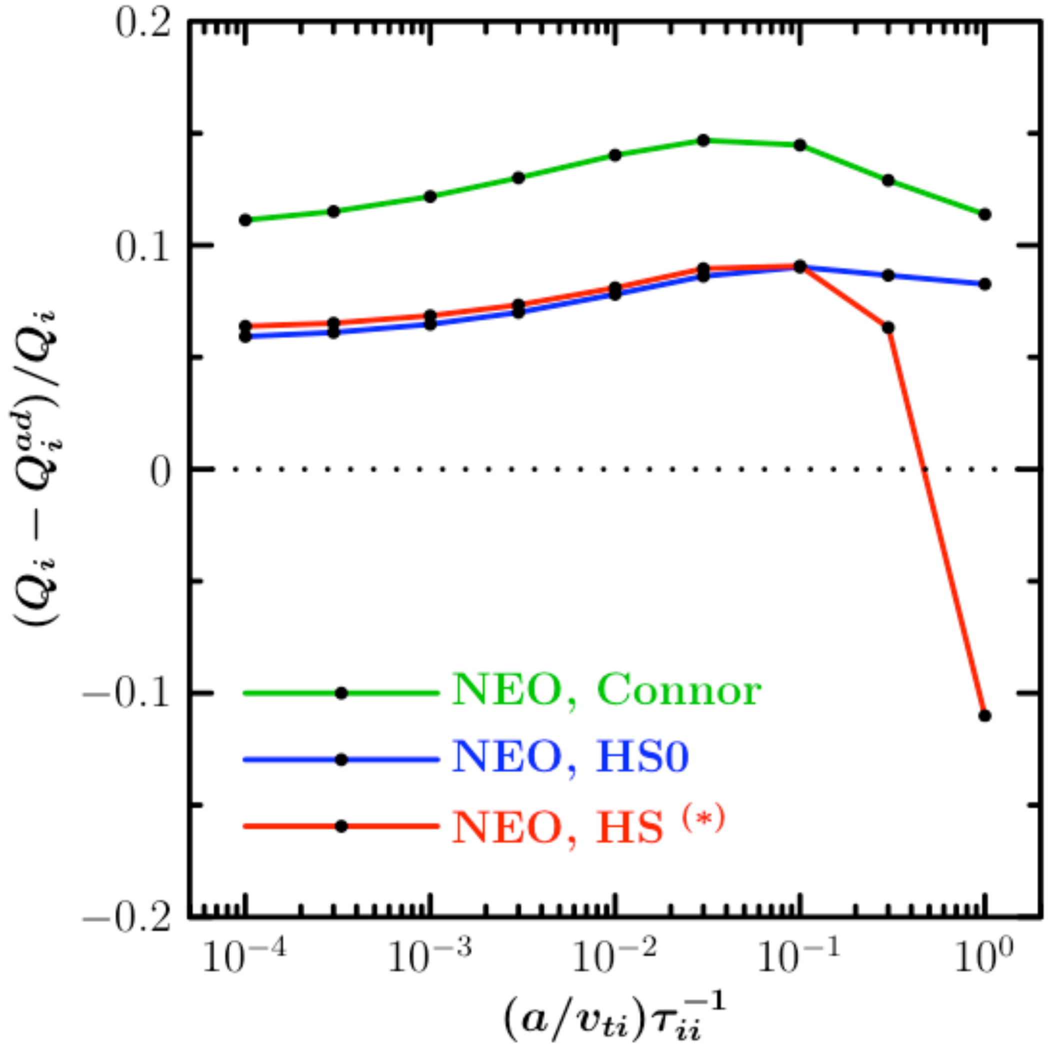
Results with self-consistent electron dynamics
Identify kinetic electron effects via comparing with ad. ele case



Kinetic electrons generally enhance Q_i by 5-10%.

1st order (poloidal) correction to the potential

Good qualitative agreement with theory.

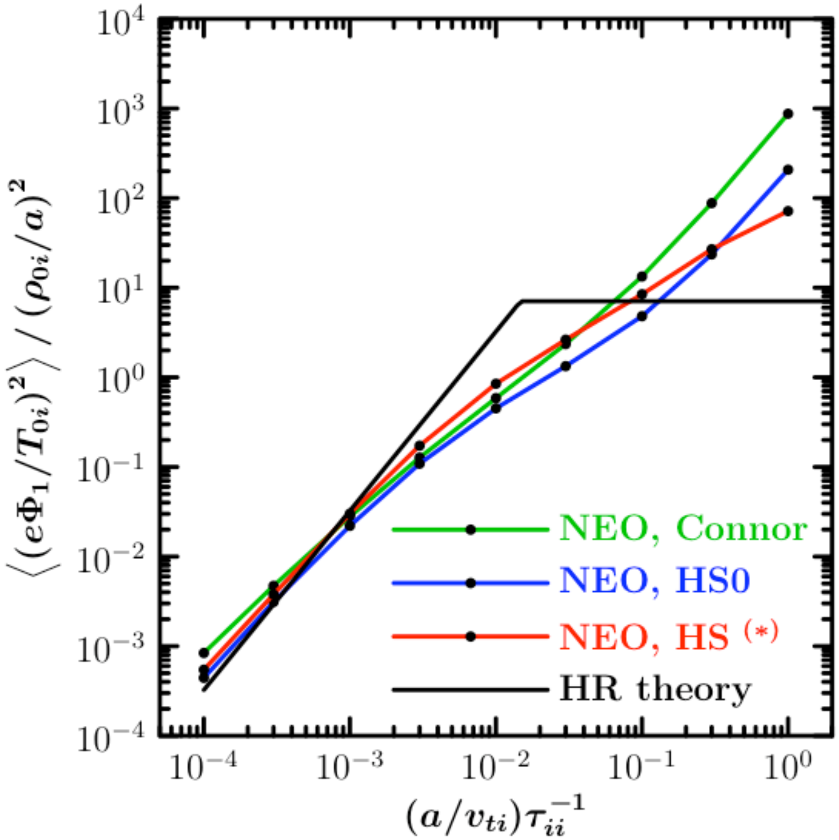
Hinton – Rosenbluth Theory:

$$\left(\frac{Z_i e}{T_{0i}} + \frac{e}{T_{0e}}\right)\left(\Phi_1 - \langle \Phi_1 \rangle\right) \sim C\varepsilon \frac{\rho_{i\theta}}{L_{Ti}} \sin\theta$$

banana regime: $C \sim 1.81\nu_{*i}$

plateau regime: $C \sim \sqrt{\pi/2}$

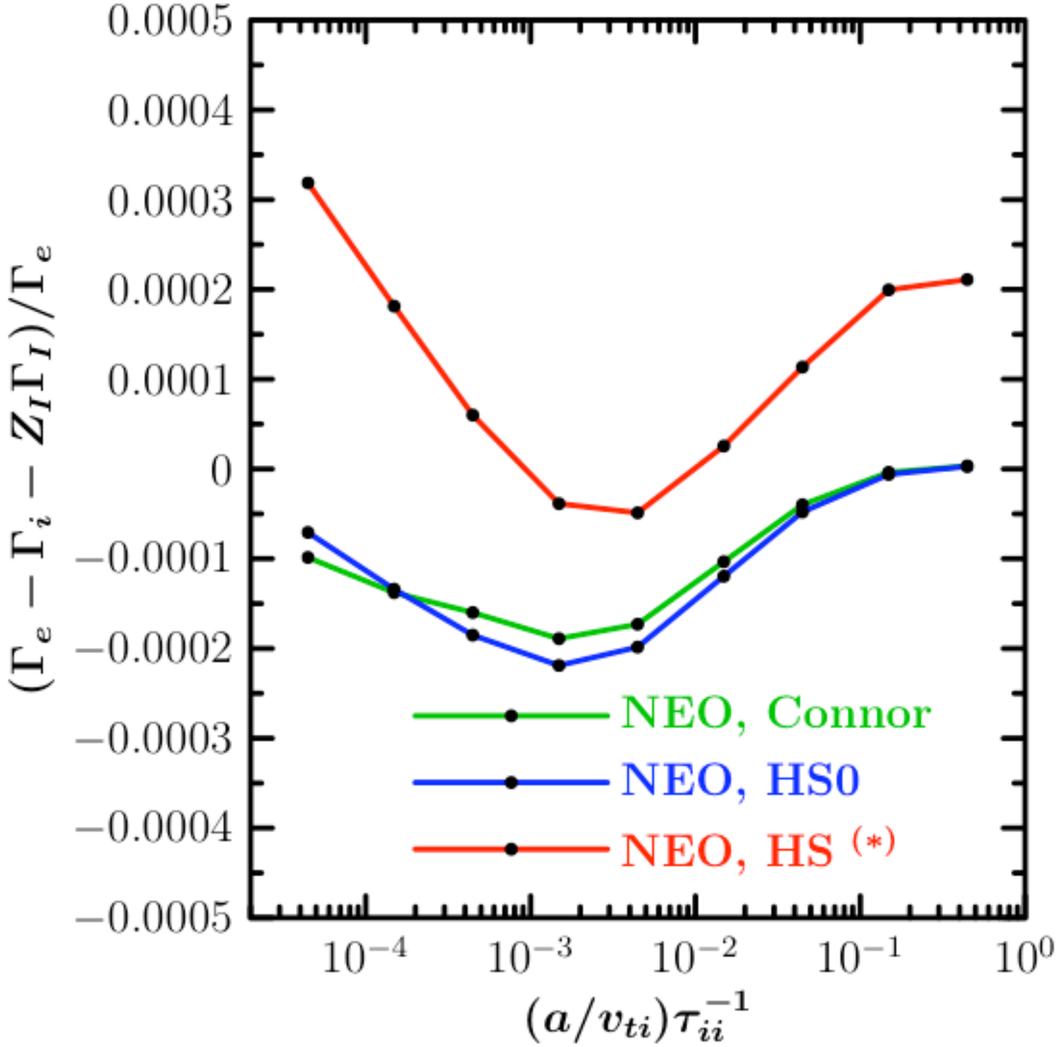
(Φ_1 makes no contribution to the particle or energy fluxes at lowest order.)



Hinton & Rosenbluth, PF 16, 836 (1973).

Impurity Dynamics

Multi-species sims : ions + eles + heavy-ion (carbon) impurities



Ambipolarity is confirmed to high accuracy.

GA standard parameters + C:
$f_I = Z_I(n_{0I}/n_{0e}) = 0.1$
$a/L_{nI} = a/L_{ni}$
$T_I = T_i$

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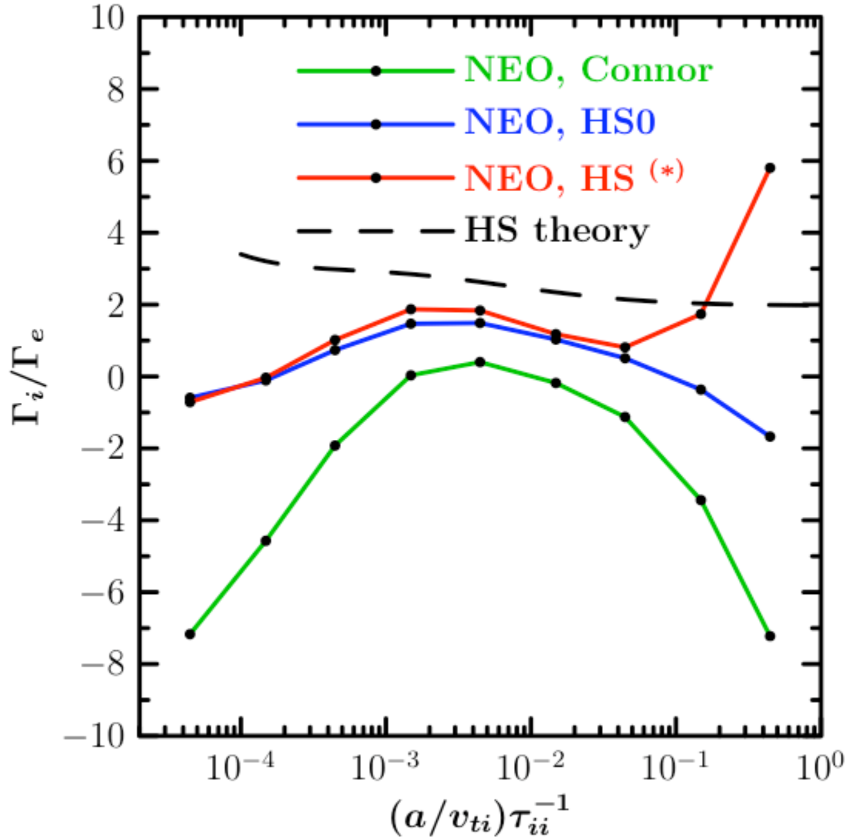
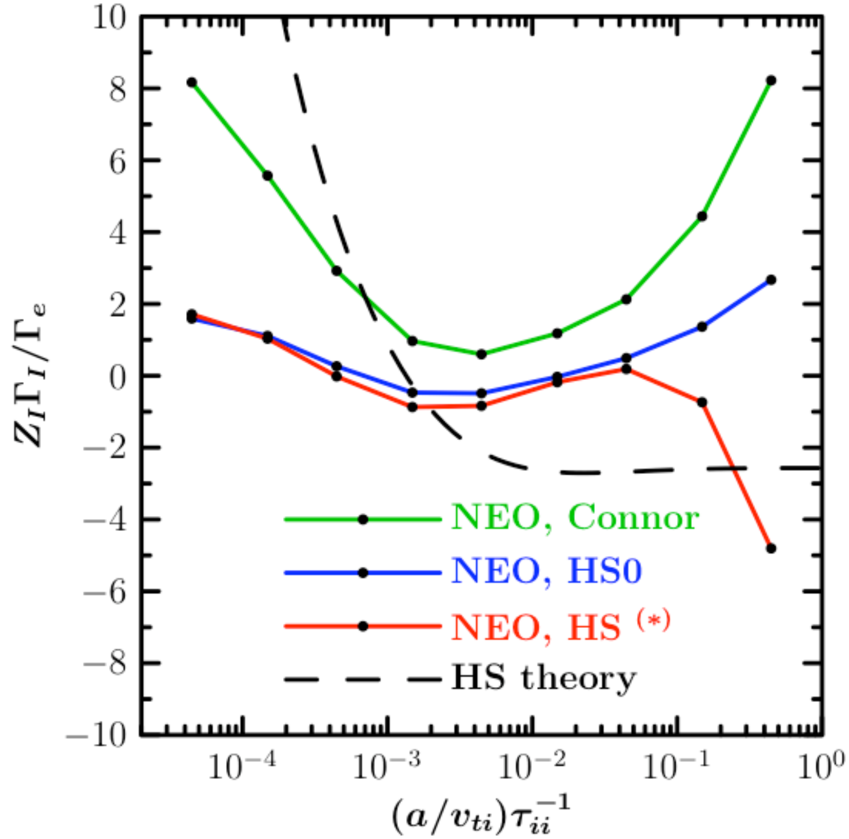
Impurity Dynamics
Comparison of 2nd order particle fluxes with analytical theory

- The multi-species analytical theory is poor.
- The Connor model is largely inaccurate.

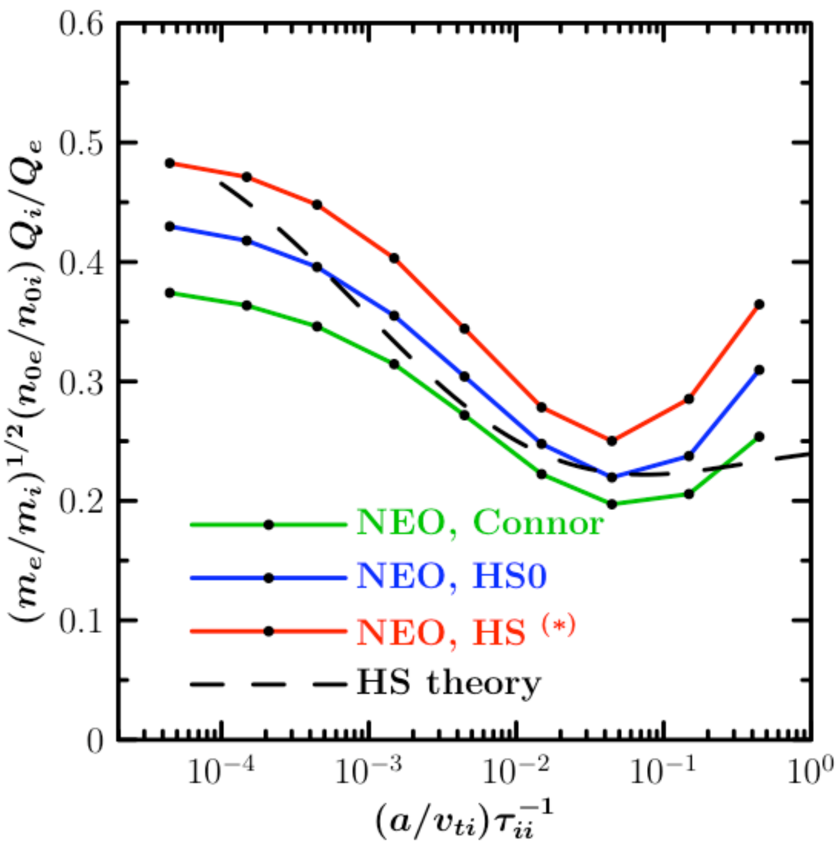


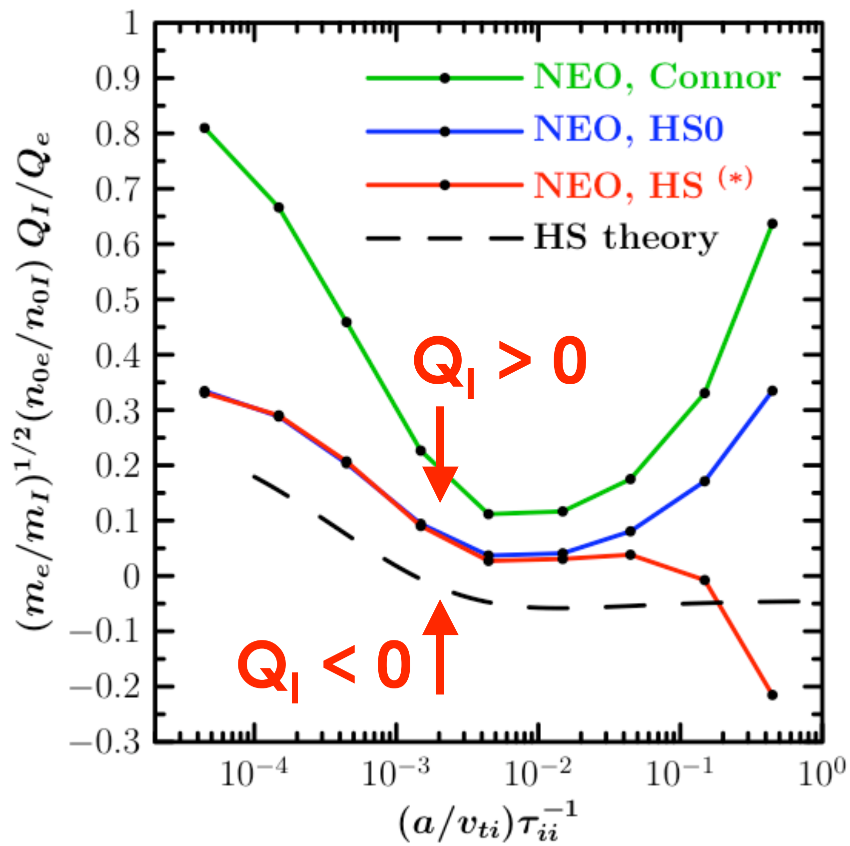


Hirshman & Sigmar, PF 20, 418 (1977).

Impurity Dynamics
Comparison of 2nd order energy fluxes with analytical theory

The analytical theory is good for Q_i but not for Q_I.





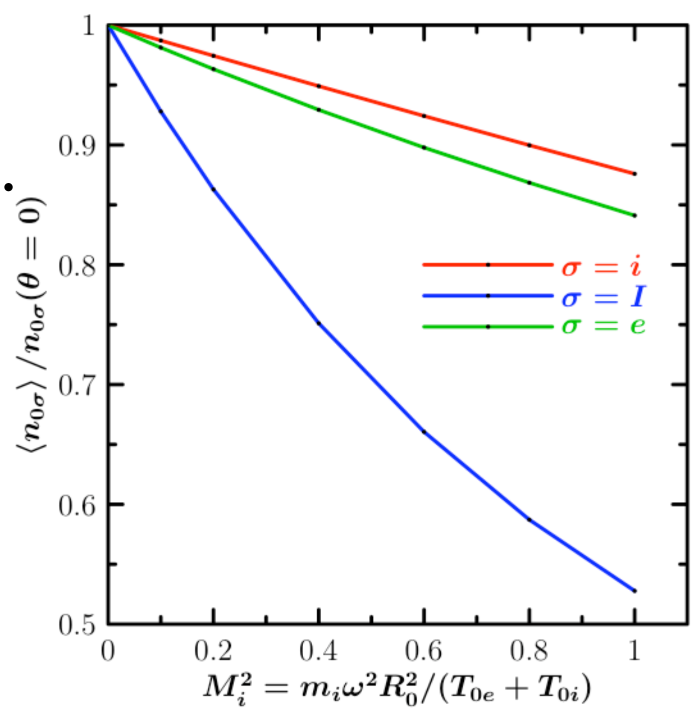
Impurity Dynamics w/ Toroidal Rotation Effects

Generalize the DKEs to allow for flow speeds ~ O(v_{th})

Following the derivation by Hinton & Wong:

$$\Phi = \Phi_{-1} + \Phi_0 + \Phi_1 + \Phi_2 + \ldots$$

$$\vec{V}_{0a} = \omega R^2 \nabla\varphi\,, \quad \omega(\psi) = -c\frac{d\Phi_{-1}}{d\psi}$$



O(1): $f_{0a} = \frac{n_{0a}}{(2\pi T_{0a}/m_a)^{3/2}} e^{-v^2/2v_{ta}^2}$ v → rotating frame speed

$$n_{0a}(\psi,\theta) = N_{0a}(\psi)\exp\left(-\frac{Z_a e}{T_{0a}}\tilde{\Phi}_0(\theta) + \frac{\omega^2 R(\theta)^2}{2v_{ta}^2}\right)$$

$$\tilde{\Phi}_0 = \Phi_0 - \langle\Phi_0\rangle$$

determined by quasi-neutrality
(solve w/ Newton's method)

formation of potential wells, which can enhance the effective fraction of trapped particles.

Hinton & Wong, PoP 28, 3082 (1985).

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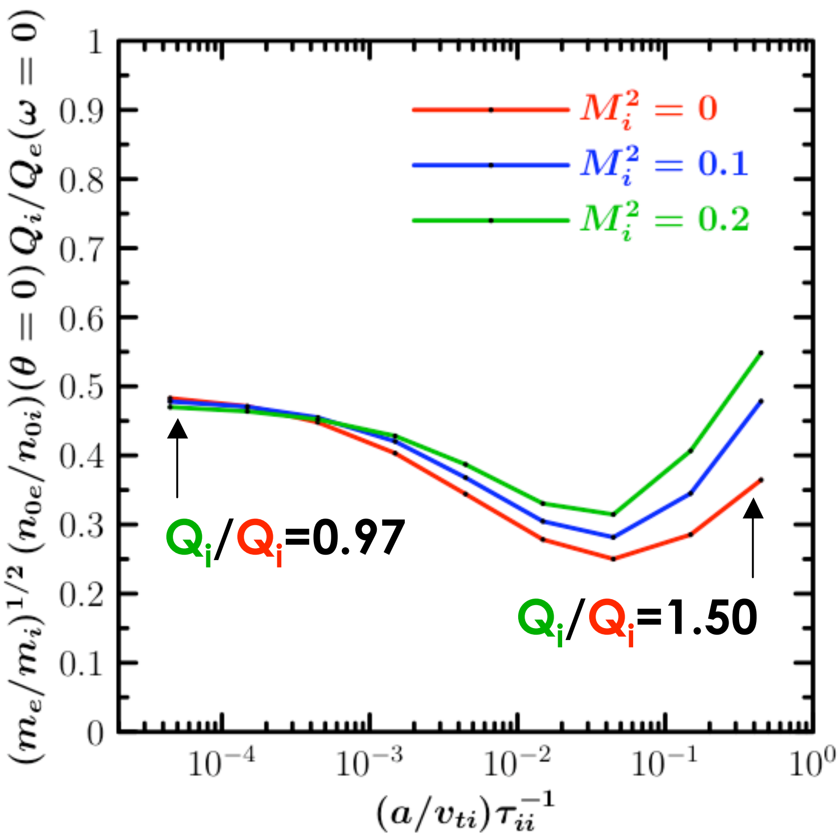
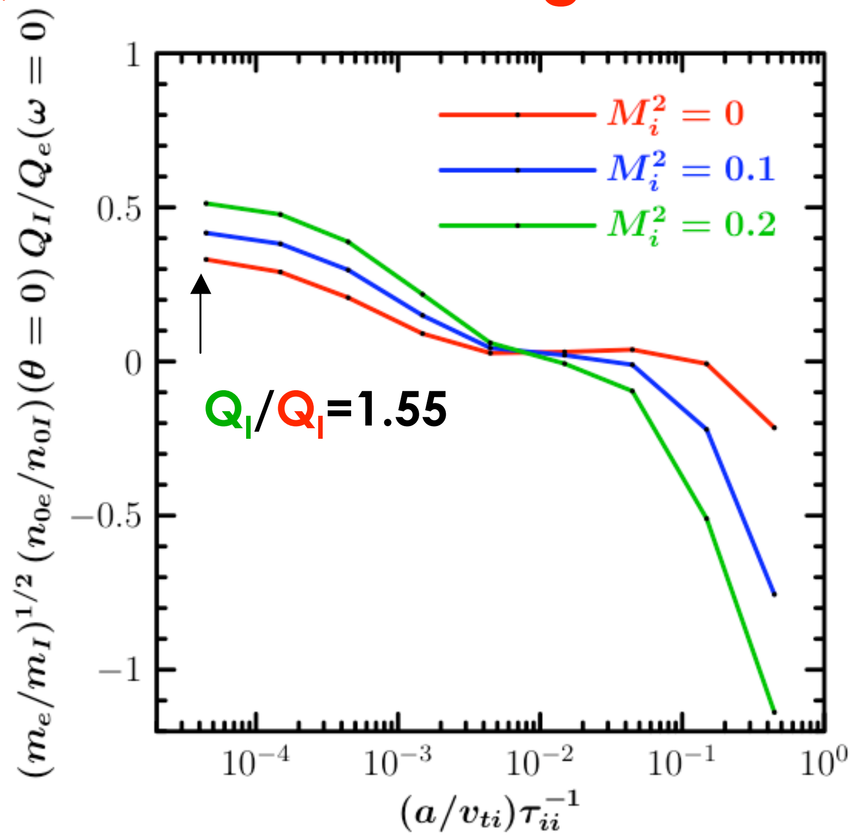
Impurity Dynamics w/ Toroidal Rotation Effects

Explore the effects of rapid toroidal rotation on Q

The effect on Q_I is stronger, but overall not significant.



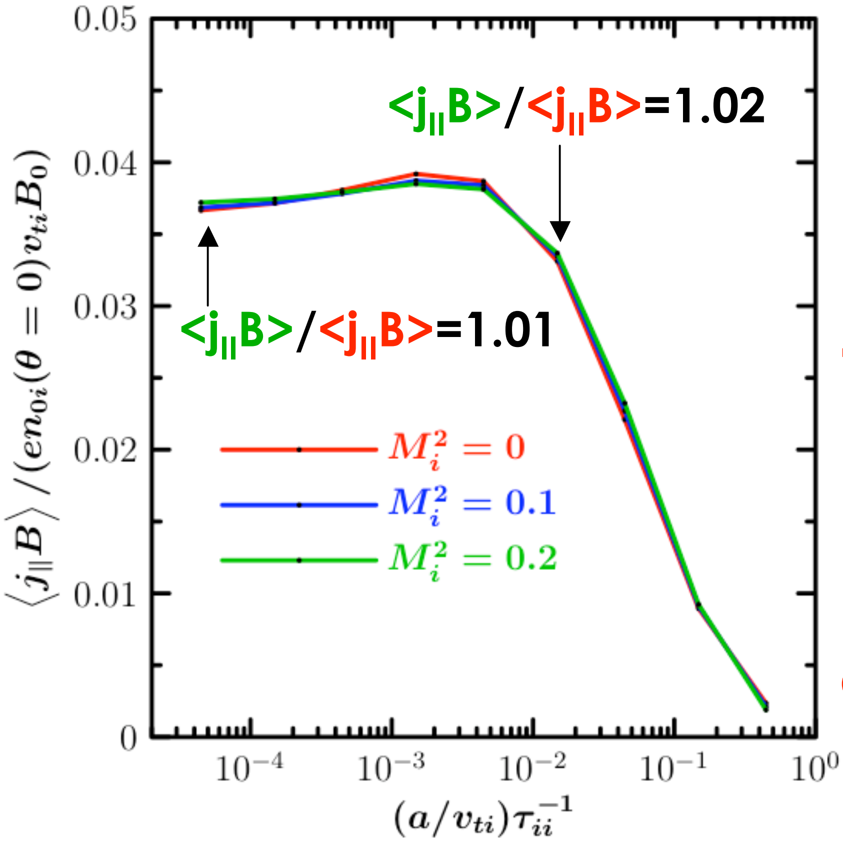


NEO results with HS collision op

Impurity Dynamics w/ Toroidal Rotation Effects

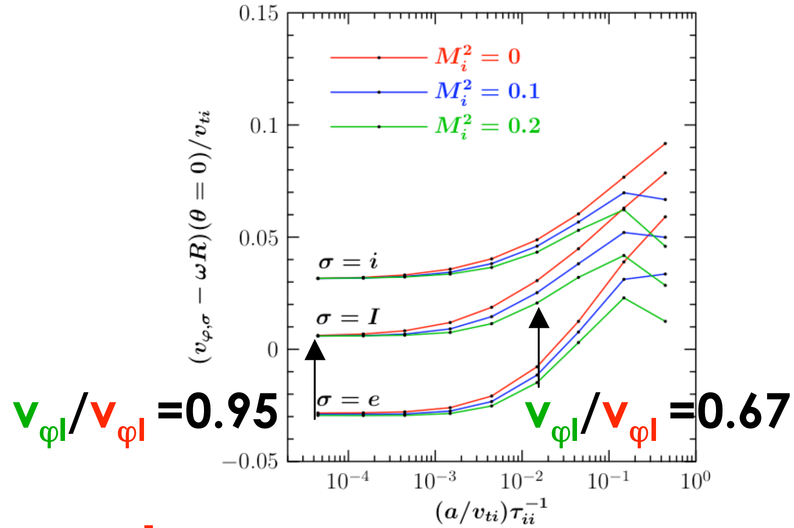
Explore the effects of rapid toroidal rotation on the flows

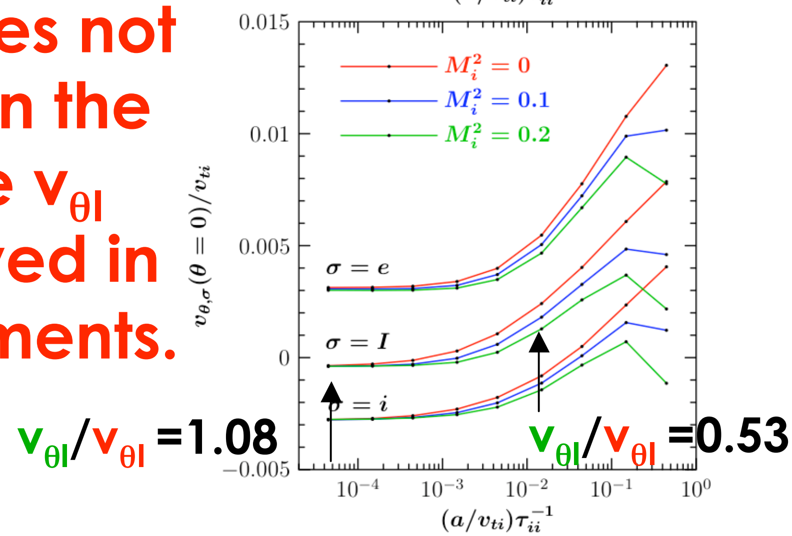
The effect on the bootstrap current is generally weak.



NEO results with HS collision op

This does not explain the large $v_{\theta I}$ observed in experiments.





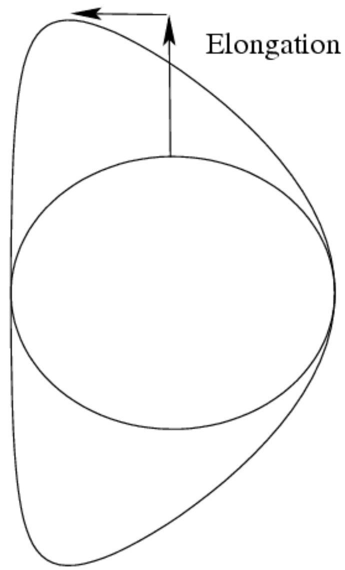
Plasma Shaping Effects
Use the Miller local equilibrium model to vary plasma shape

Miller Equilibrium:

- Nine parameters are required to fully describe the local equilibrium:
  $\{\kappa, \delta, \partial_r\kappa, \partial_r\delta, s, \partial_r\beta_{unit}, q, R_0/a, \partial_r R_0\}$

- Flux surface shape is specified using a standard formula for D-shaped plasmas

- B_{unit} is a free parameter: $\dfrac{\partial\psi}{\partial r} = \dfrac{r}{q} B_{unit}$



Vary κ and δ at fixed ρ_{unit}: $\rho_{i,unit} \doteq \dfrac{v_{ti}}{Z_i e B_{unit} / m_i c}$

Miller et al, PoP 5, 973 (1998).

GENERAL ATOMICS

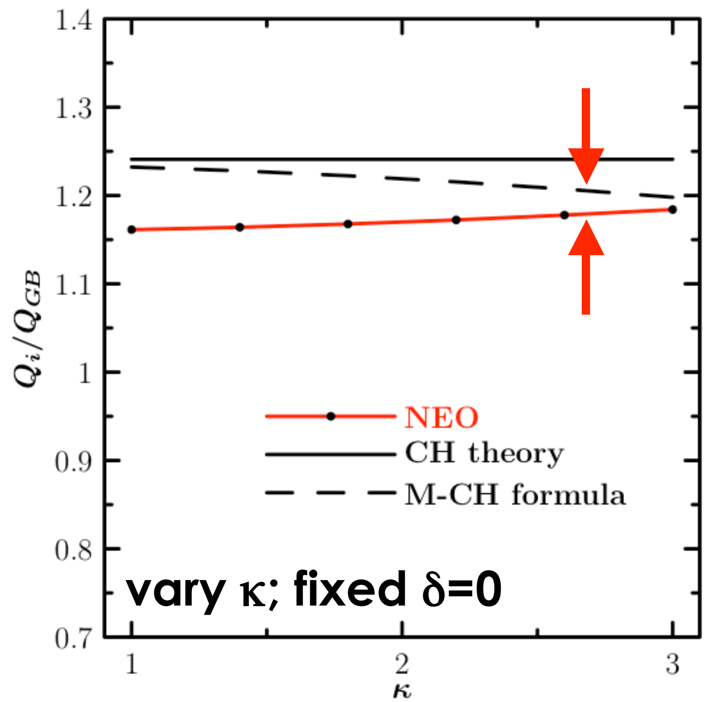
Plasma Shaping Effects

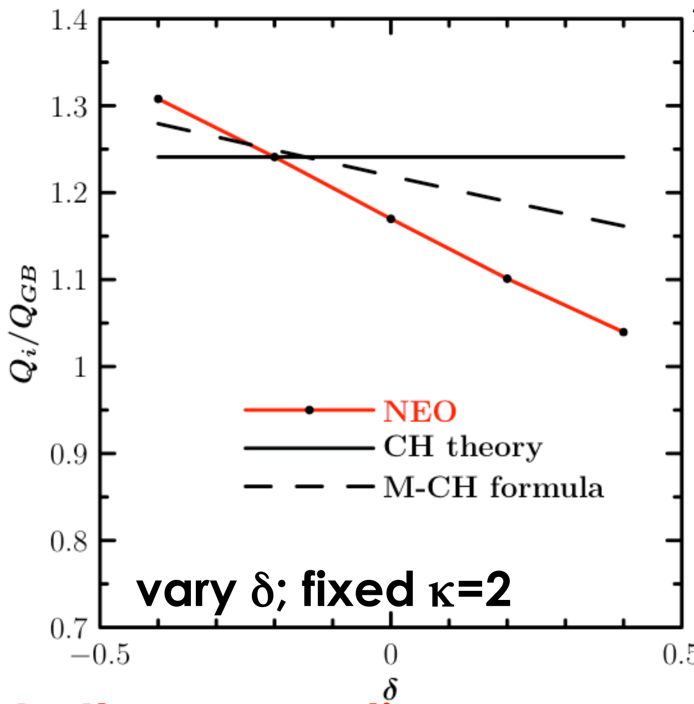
Explore the interpretation of the Chang-Hinton theory for shaped plasmas

$$\frac{Q_i}{n_{oi}T_{oi}} = -1.32\sqrt{\varepsilon}\,\tau_i^{-1}\left(\frac{q}{\varepsilon}\right)^2 \rho_{i,unit}^2 \left[\frac{E}{1+1.03\sqrt{\nu_{*i}}+0.31\nu_{*i}} + \frac{F(1.77)\nu_{*i}\varepsilon^{3/2}}{1+0.74\nu_{*i}\varepsilon^{3/2}}\right]\frac{\partial \ln T_{0i}}{\partial r}$$

$$E = \frac{0.66+1.88\sqrt{\varepsilon}-1.54\varepsilon}{0.66}\left\langle\frac{B_0^2}{B^2}\right\rangle$$

$$F = \frac{1}{2\sqrt{\varepsilon}}\left(\left\langle\frac{B_0^2}{B^2}\right\rangle - \left\langle\frac{B^2}{B_0^2}\right\rangle^{-1}\right)$$





adiabatic ele

$(a/v_{ti})\tau_{ii}^{-1}=0.01$

- **Must use B_{unit} to compute the gyroradius**
- **Not valid to use B(θ) to compute the magnetic field averages**

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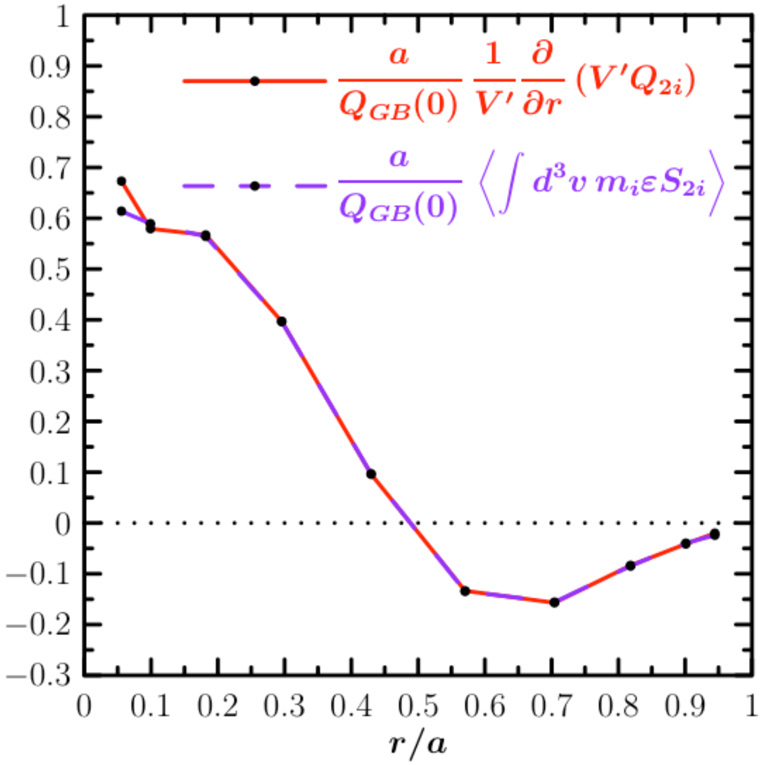
Finite Orbit Width Effects

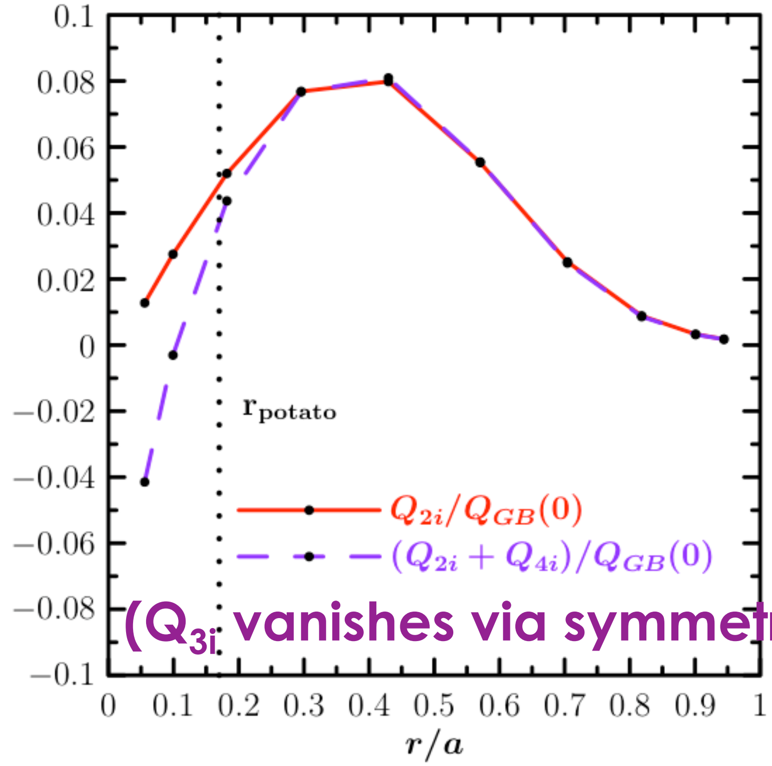
Solution of the higher-order DKEs

Verification of s.s. transport relation

$$\frac{1}{V'}\frac{\partial}{\partial r}(V'Q_{2a}) + Z_a e\frac{\partial\Phi_0}{\partial r}\Gamma_{2a} = \left\langle\int d^3v m_a \varepsilon S_{2a}\right\rangle$$



Deviations from Q_{2i} identify the break-down of the δf formalism



(Q_{3i} vanishes via symmetry)

Global Parameters: R_0= 4 m   q = 3 $(n_{0i},T_{0i}) \sim c_1+c_2 \exp(-c_3(r/a)^3)$
(s-α geometry)   a = 1m B_0 = 4 T   adiabatic ele

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Conclusions

NEO provides a first-principles DKP-based calculation of the neoclassical transport coefficients.

- **Verification/analytical comparisons**: Demonstrated agreement with the Taguchi model for the full HS collision op. Confirmed that C-H theory overestimates Q_i for intermediate ε.
- **Ambipolarity**: Confirmed for multi-species plasmas.
- **Potential correction**: Computed for 1st order. Found qualitative agreement with analytical theory.
- **Impurity transport** (heavy-ions): Showed that the H-S theory gives a poor prediction of ion and impurity fluxes.
- **Rotation effects**: Generally weak.
- **Shaping studies**: Found a weak effect in κ (stronger in δ). Showed that modified C-H theory based on $B(\theta)$ is not accurate.
- **FOW effects**: Higher-order solution identified the break-down of the δf formalism near $r_{potato} \Rightarrow$ requires full F.