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
  - Finite-orbit-width 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

NEO solves a hierarchy of equations based on an 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

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

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

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

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

Standard neoclassical

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

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

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

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

$$+ \frac{Z_a e}{m_a}\left(v_\parallel \hat{b}\cdot\nabla\Phi_1 + \vec{v}_D\cdot\nabla\Phi_0\right)\frac{\partial f_{1a}}{\partial\varepsilon} + \dot{\mu}\frac{\partial f_{1a}}{\partial\mu} + S_{2a}\ *$$

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

*** required for solvability**

Finite-obit-width correction

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

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

The ambipolarity relation, which requires complete cross-species collisional coupling, is preserved.

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

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

$$\Downarrow$$

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

$$f_{1a} = g_{1a} - f_{0a} \frac{Z_a e}{T_{0a}} \Phi_1$$

$$I(\psi) = R B_t$$

ψ : poloidal flux / (2π)

$$\frac{I}{\psi'} \rightarrow \frac{q R_0}{r} \quad \text{(s - } \alpha \text{ geometry)}$$

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

Three model forms of the linearized collision operator are implemented and compared.

- **Connor Model**

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

- **Zeroth Order Hirshman-Sigmar Operator**

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

- **Full Hirshman-Sigmar Operator**

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

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

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

The NEO algorithm is highly accurate and time efficient.

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

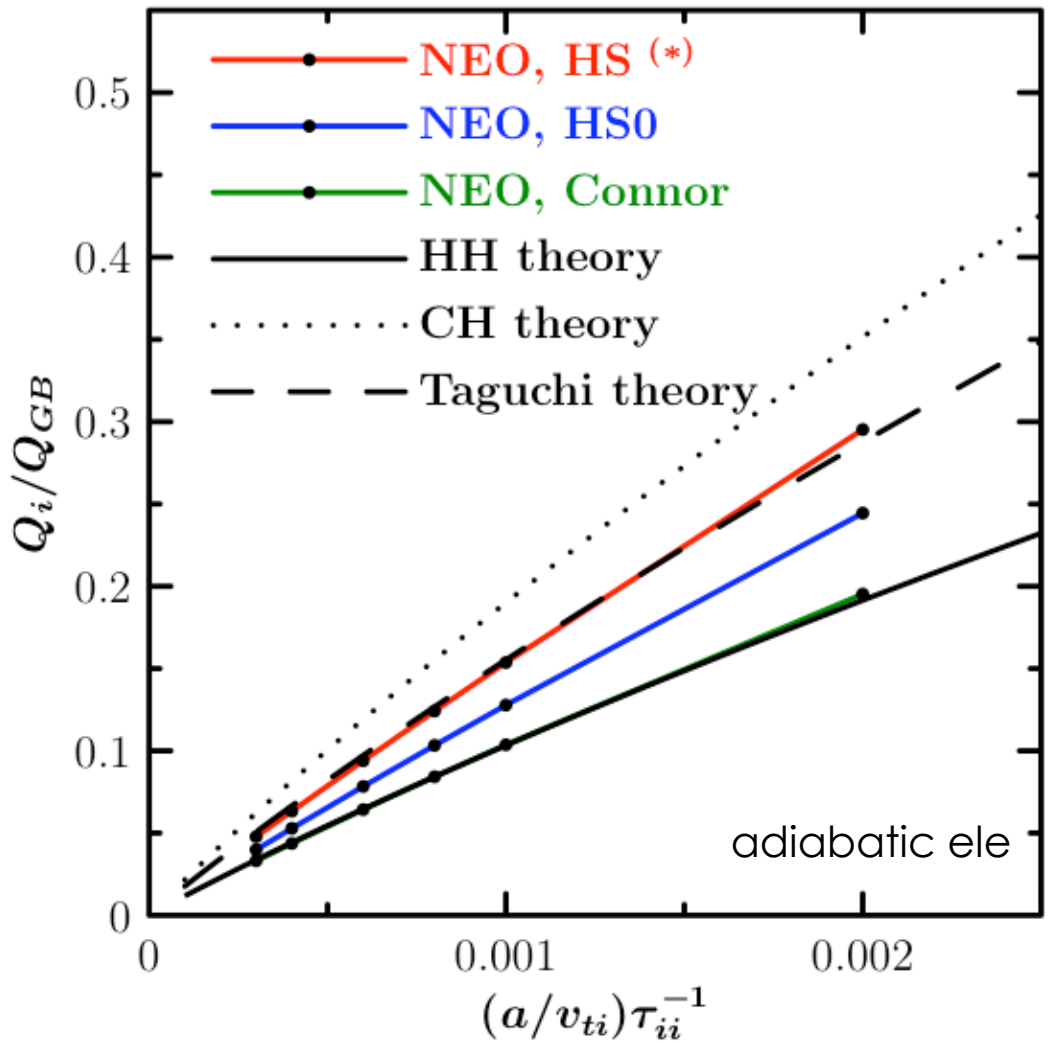
$$f_{ka} = g_{ka} - f_{0a}\frac{Z_a e}{T_{0a}}\Phi_k$$

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

Typical sim time is < 1min.

Verification: With the full HS collision op, NEO recovers Taguchi's theory, which is the most accurate analytic result in the banana regime.



The Connor & HS0 collision ops underestimate Q_i.

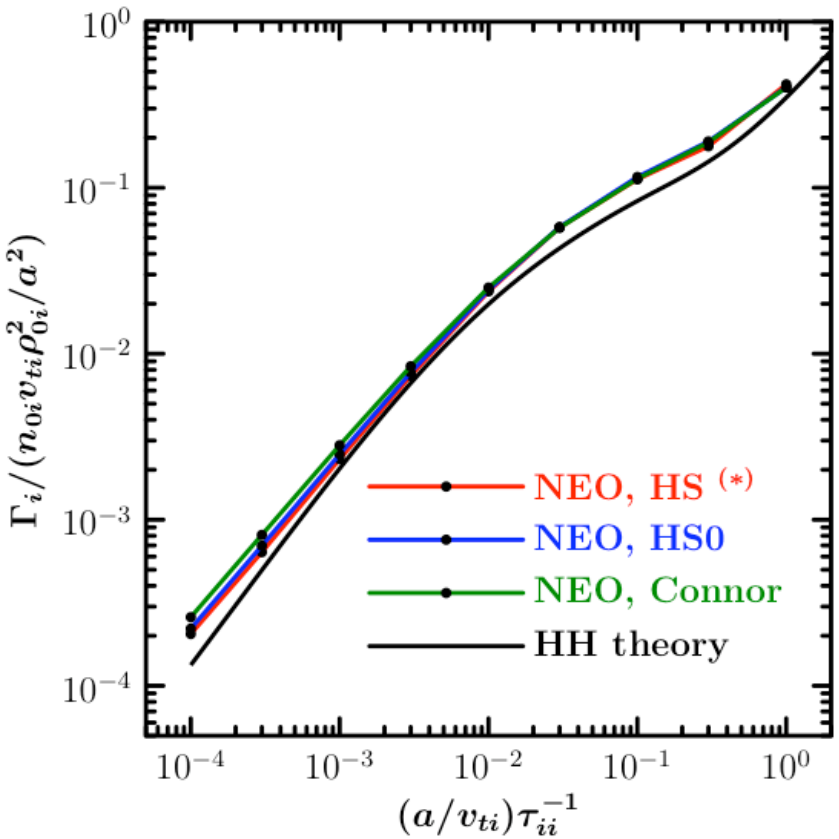
Chang-Hinton theory overestimates Q_i.

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

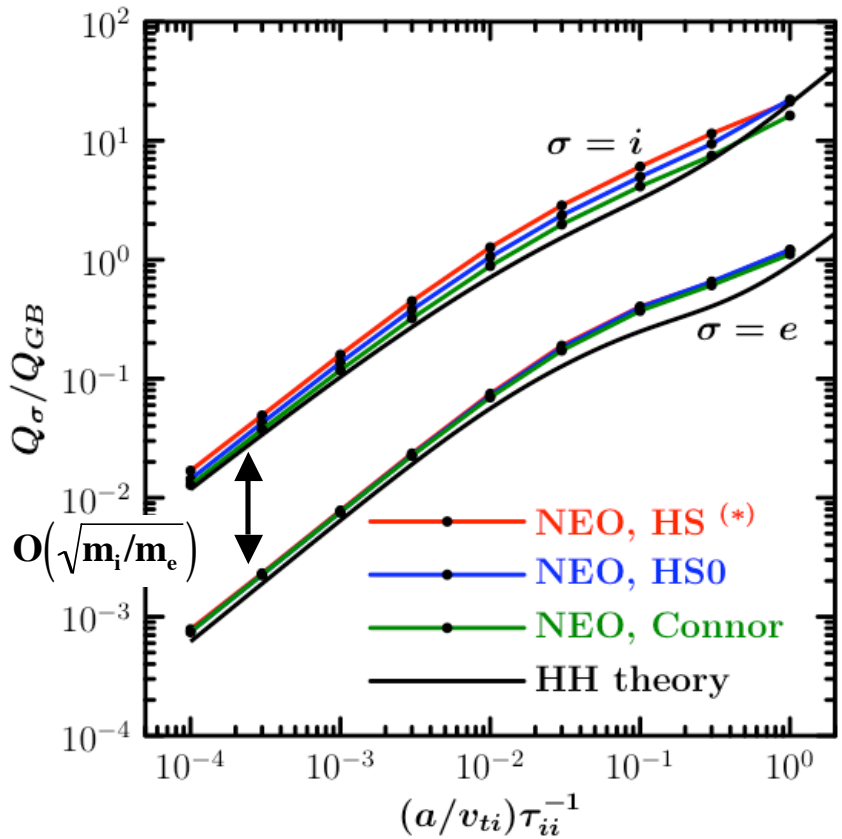
Hinton & Hazeltine, RMP 48, 239 (1976).
Chang & Hinton, PF 25, 1493 (1982).
Taguchi, PPCF 30, 1897 (1988).

With self-consistent electron dynamics, the 2nd order fluxes have been successfully benchmarked with analytic theory.

Ambipolarity is confirmed.

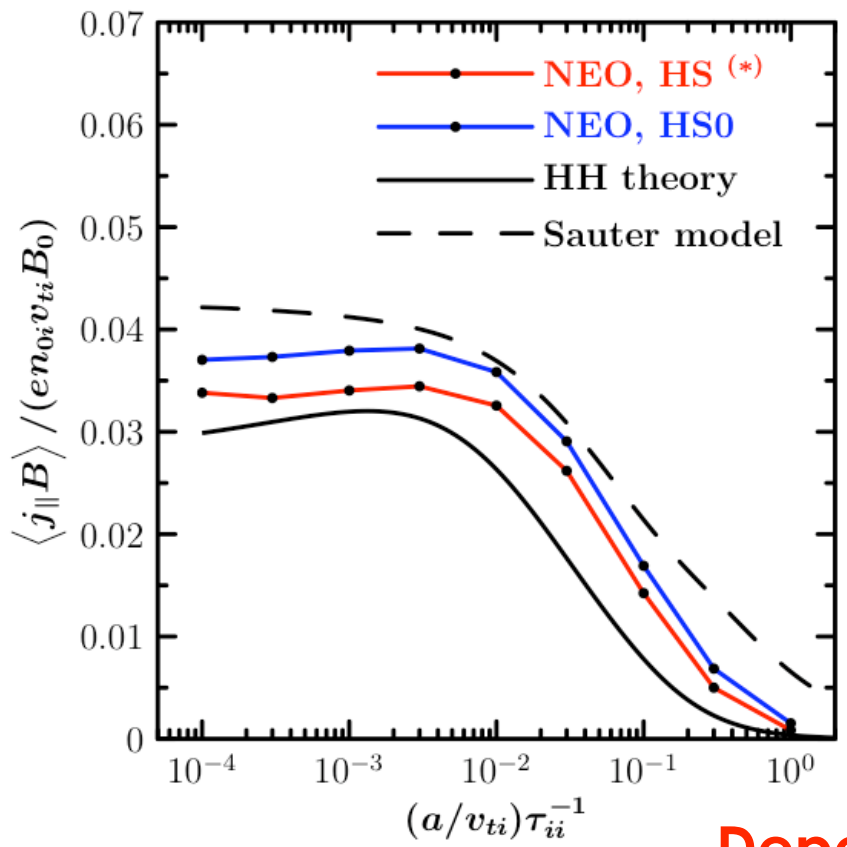


The Connor & HS0 collision ops consistently underestimate Q.



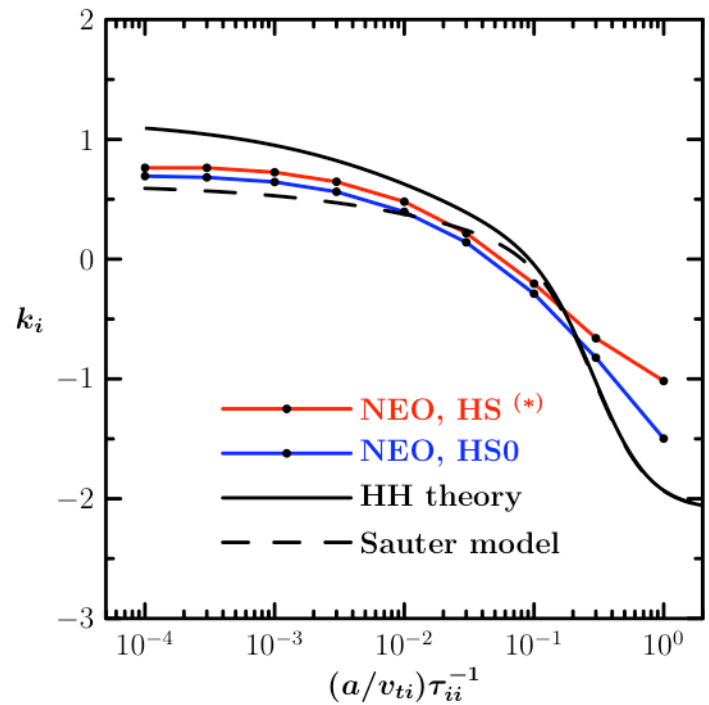
Full electron-deuterium mass ratio used.

With NEO, we find that the Sauter model overestimates the bootstrap current.



Standard neoclassical relation:

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



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

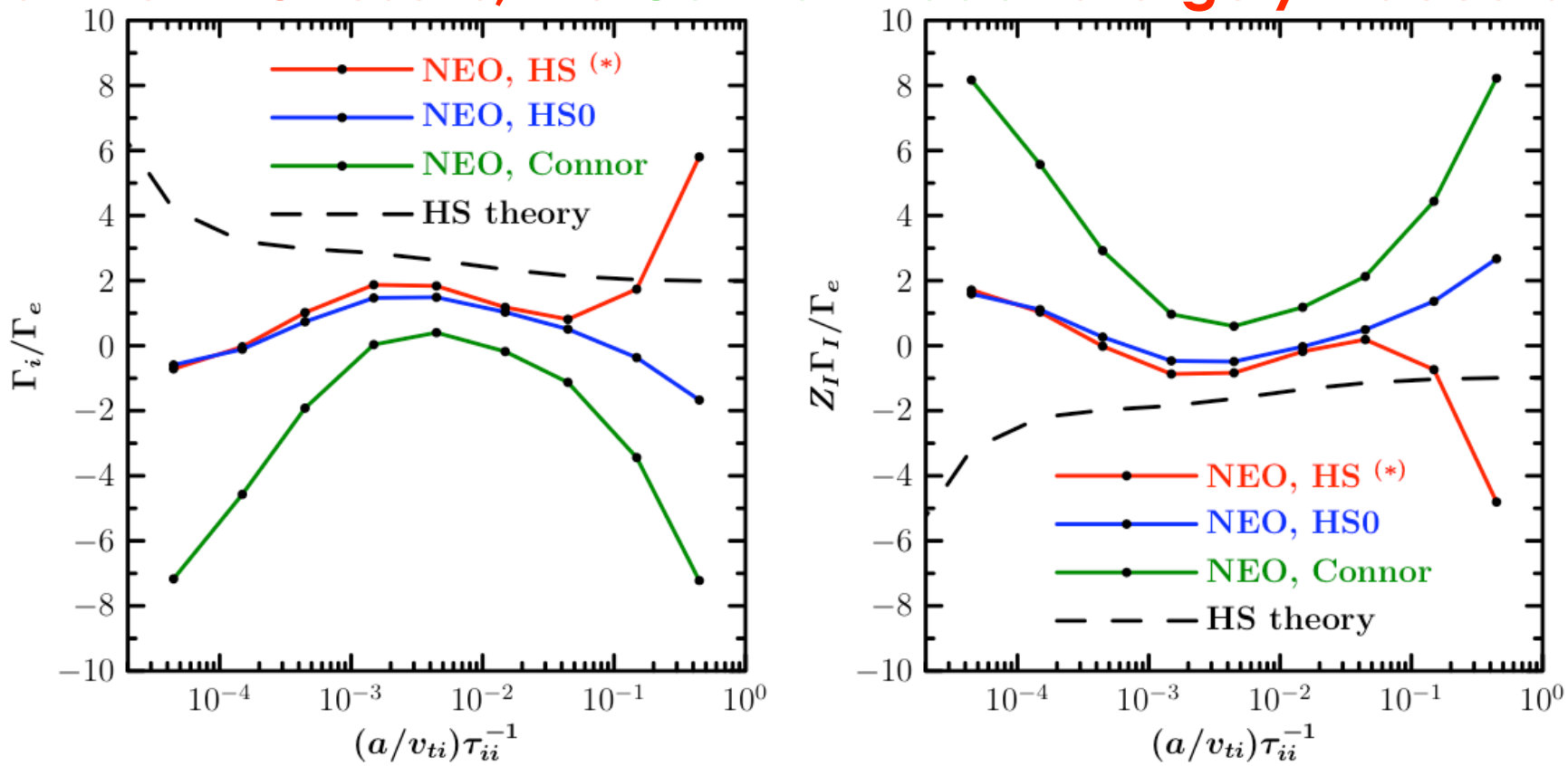
Hinton & Hazeltine, RMP 48, 239 (1976).

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

Studies of the effects of impurities find that the HS multi-species analytic theory is poor.

Comparison of 2nd order particle fluxes with analytic theory

For the NEO results, the Connor model is largely inaccurate.

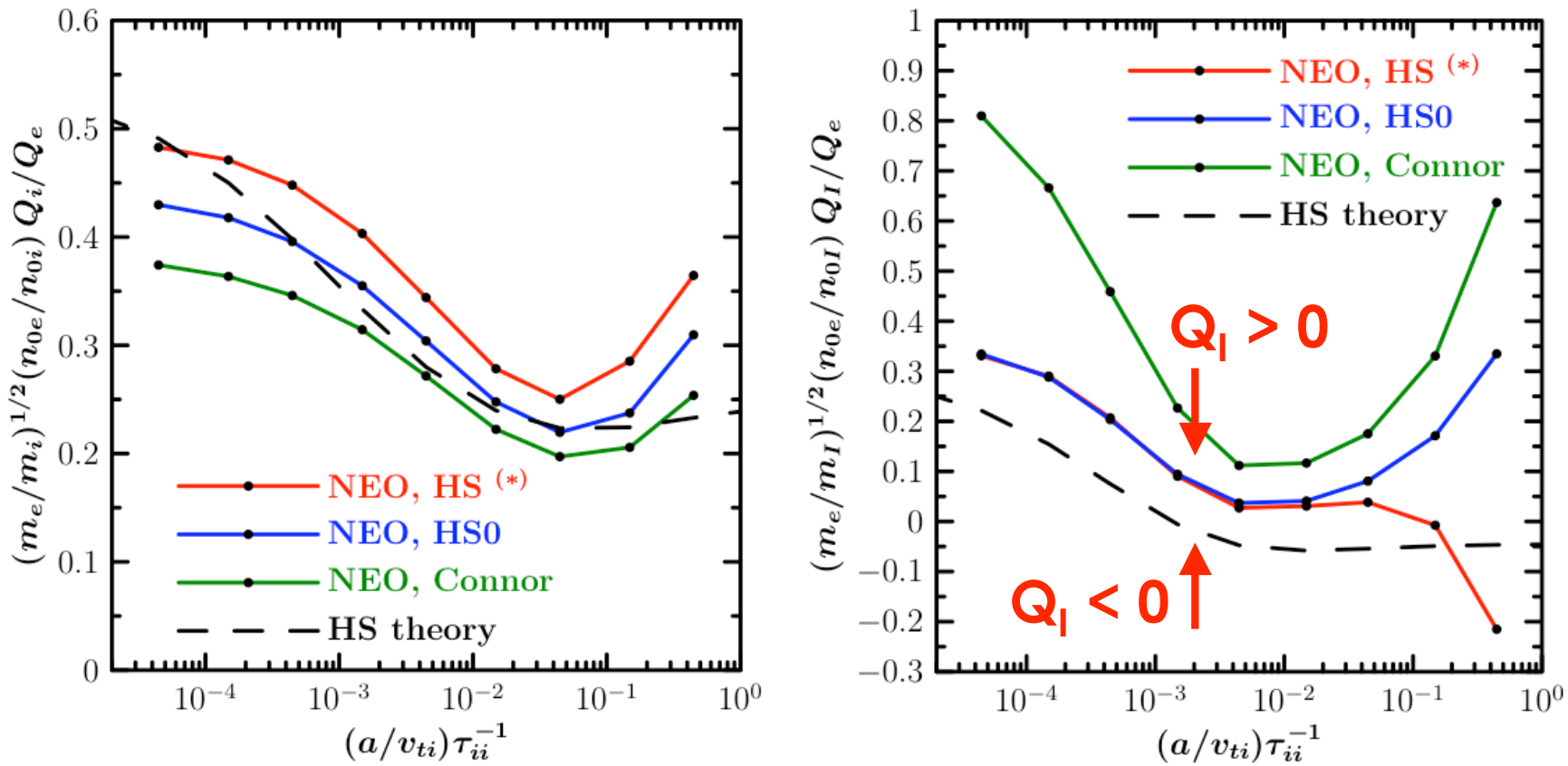


GA standard parameters + Carbon: $Z_I n_{0I}/n_{0e}=0.1$, $T_I=T_i$

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

The multi-species analytic theory is qualitatively better for Q_i but still poor for Q_I.

Comparison of 2nd order energy fluxes with analytic theory



GENERAL ATOMICS

The effects of rapid toroidal rotation, which introduces 0th-order density asymmetries, are also included in NEO.

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

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

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

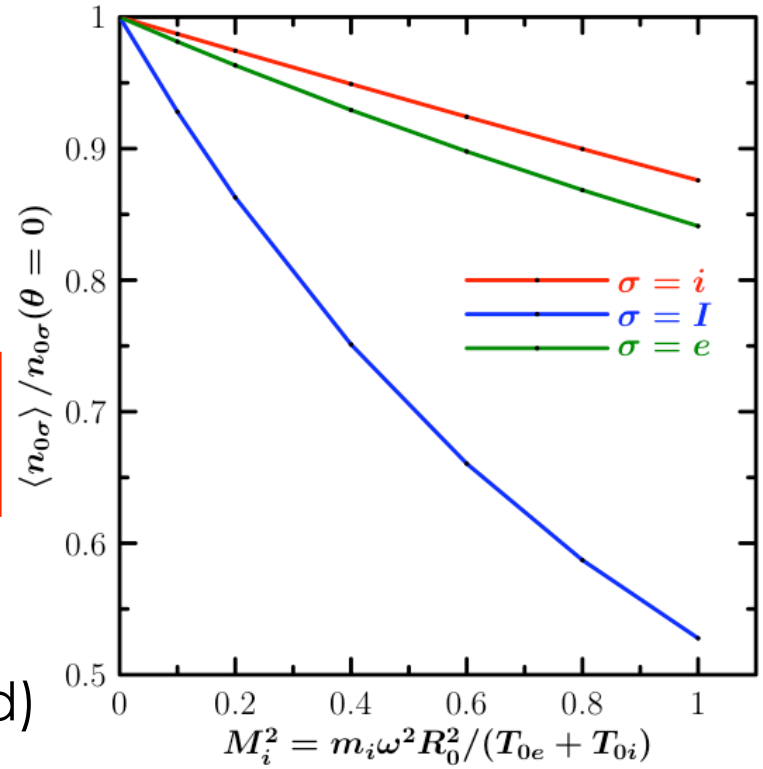
O(1): $f_{0a} = \dfrac{n_{0a}}{(2\pi T_{0a}/m_a)^{3/2}} e^{-v^2/2v_{ta}^2}$ v → rotating frame speed

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

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

determined by quasi-neutrality

(solve w/ Newton's method)

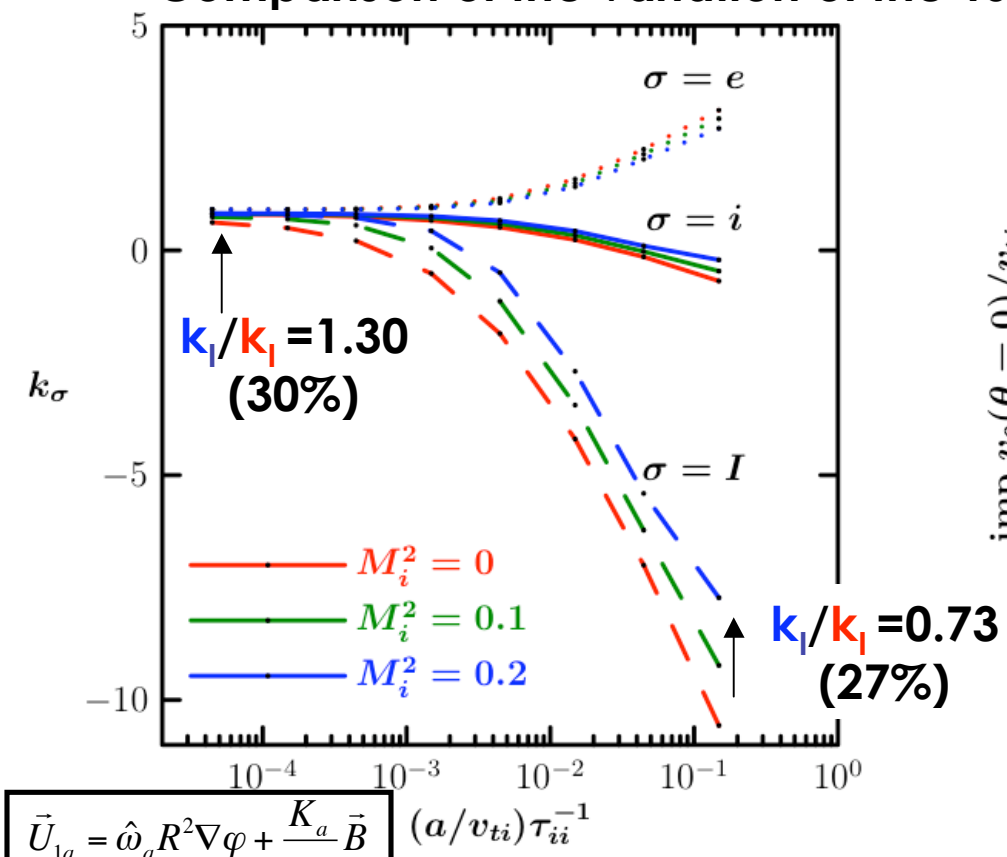


formation of potential wells, which can enhance the effective fraction of trapped particles.

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

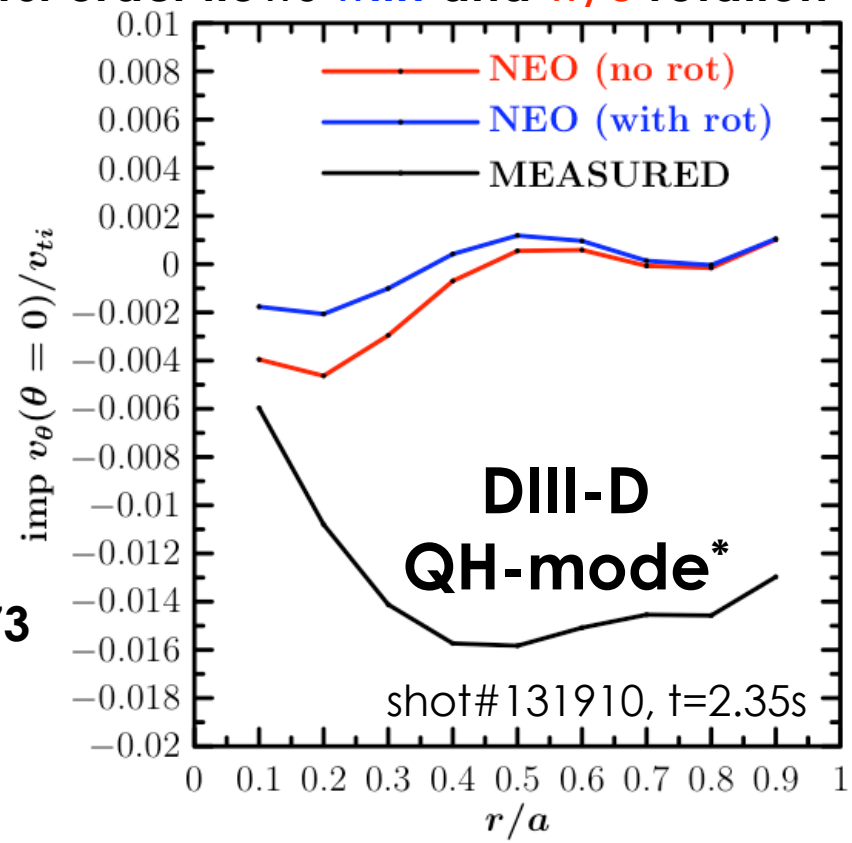
The effects of toroidal rotation are weak in typical experiments.

Comparison of the variation of the 1st order flows with and w/o rotation



$$\vec{U}_{1a} = \hat{\omega}_a R^2 \nabla\varphi + \frac{K_a}{n_{0a}}\vec{B}$$

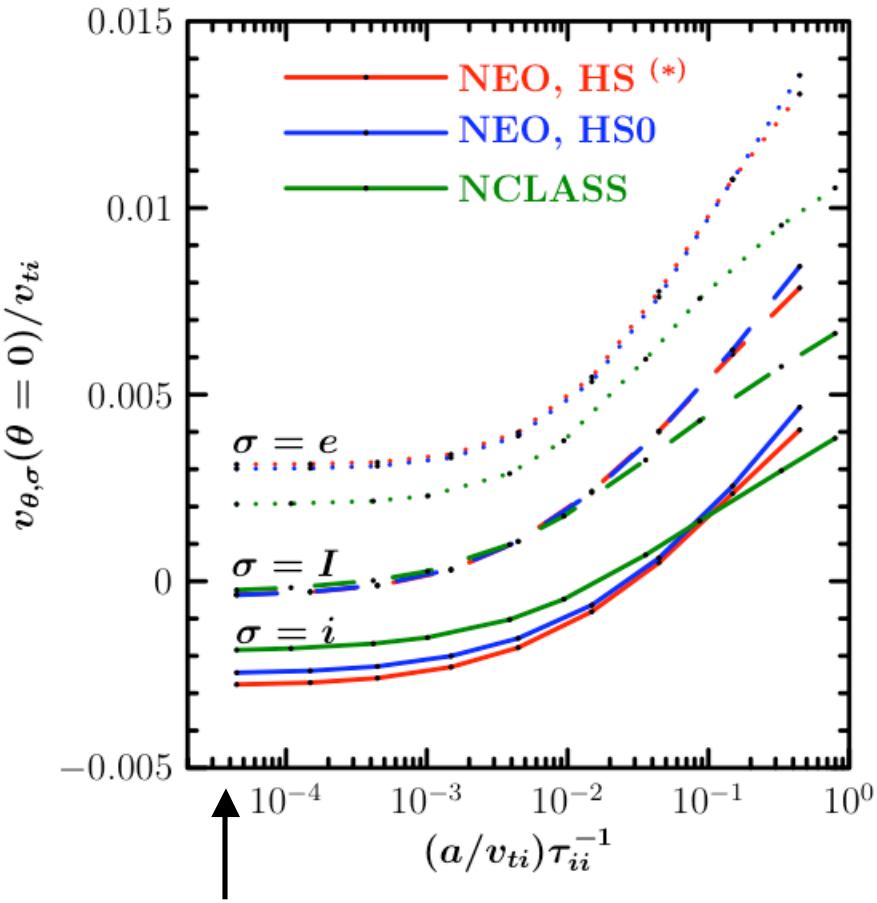
$$K_a = -k_a\left(\frac{cT_{0a}I}{Z_a e L_{Ta}\psi'\langle B^2/n_{0a}\rangle}\right), \quad \hat{\omega}_a = -\left(\frac{cT_{0a}}{Z_a e\psi'}\right)\left[\frac{d\ln p_{0a}}{dr} + \frac{z_a e}{T_{0a}}\frac{d\langle\Phi_0\rangle}{dr}\right]$$

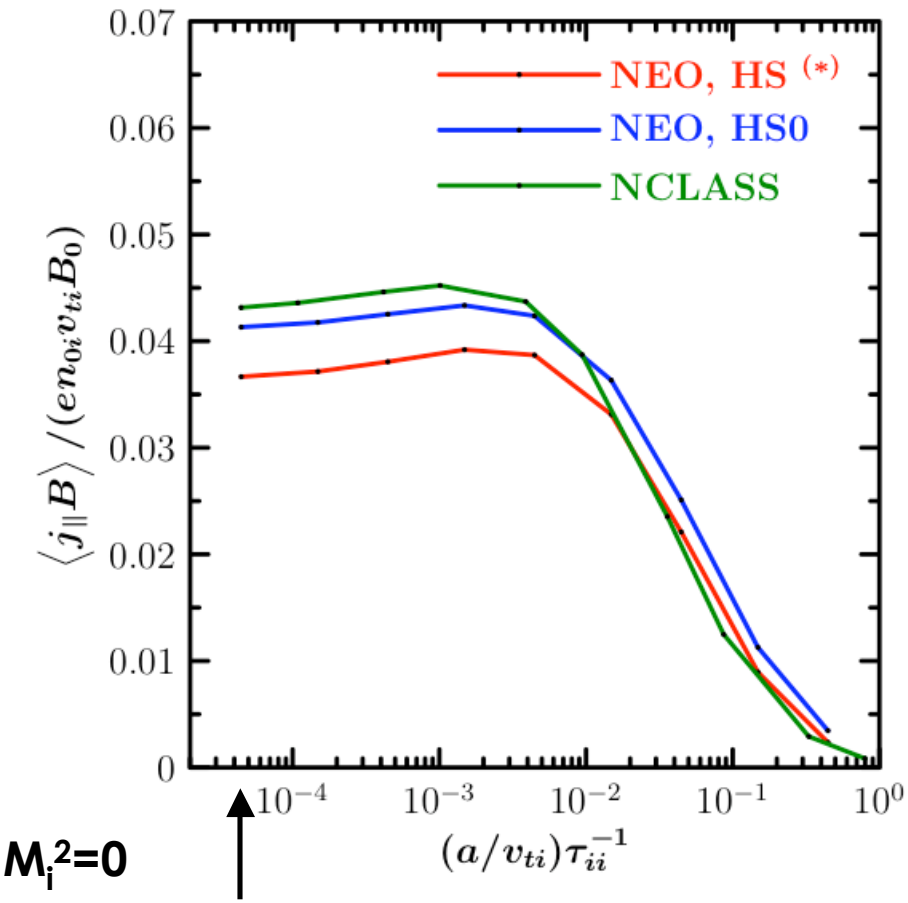


* Experimental data is being re-analyzed for accuracy.

GENERAL ATOMICS

Good overall agreement is found between NEO and NCLASS, although NCLASS slightly underestimates $|v_{pol}|$.





$M_i^2=0$

~30% difference

~17% difference

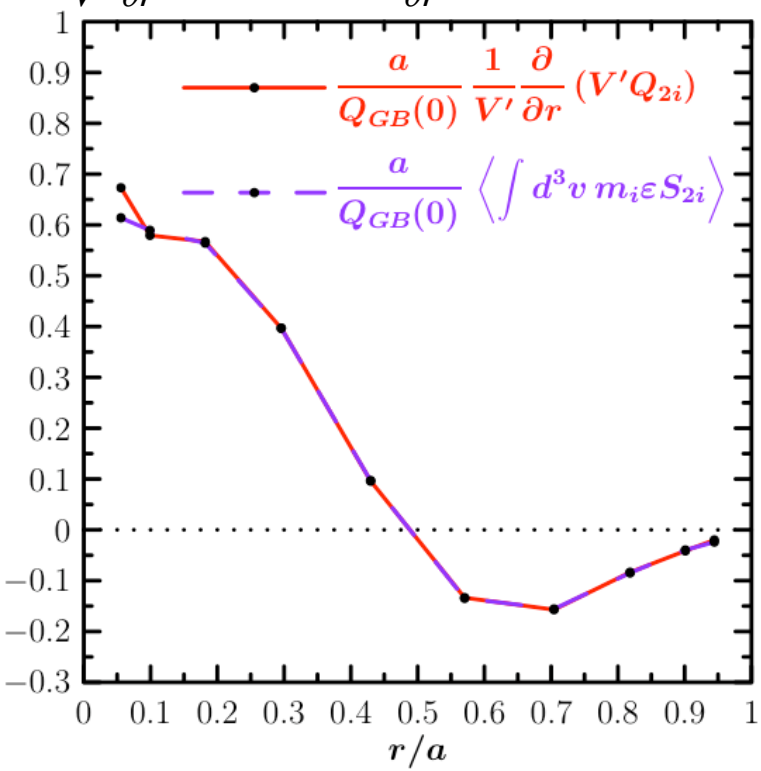
GENERAL ATOMICS

Higher-order solution of the DKEs identifies a break-down of the δf formalism due to FOW effects in the region r < r_{potato}.

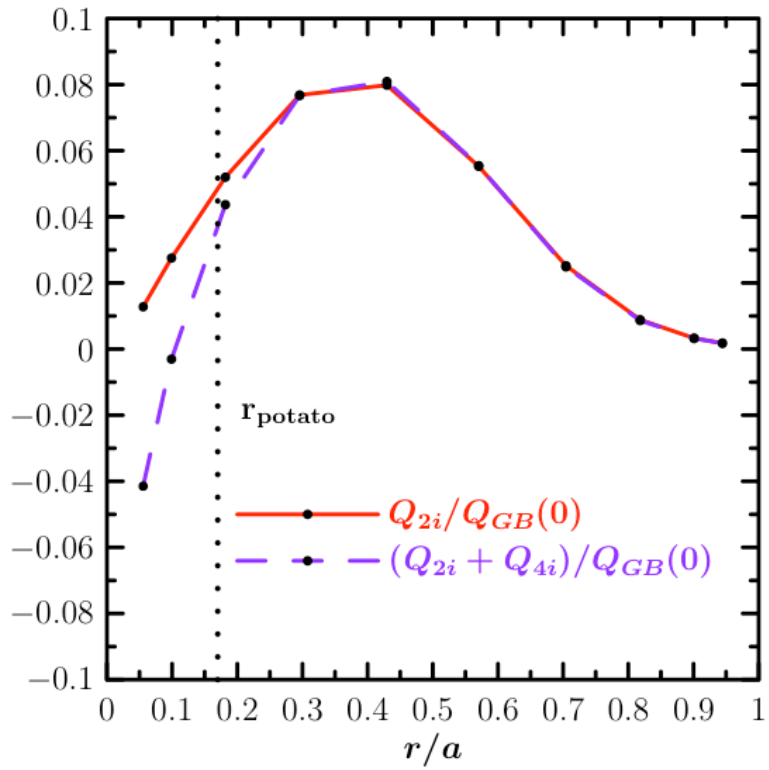
Consistency check:

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



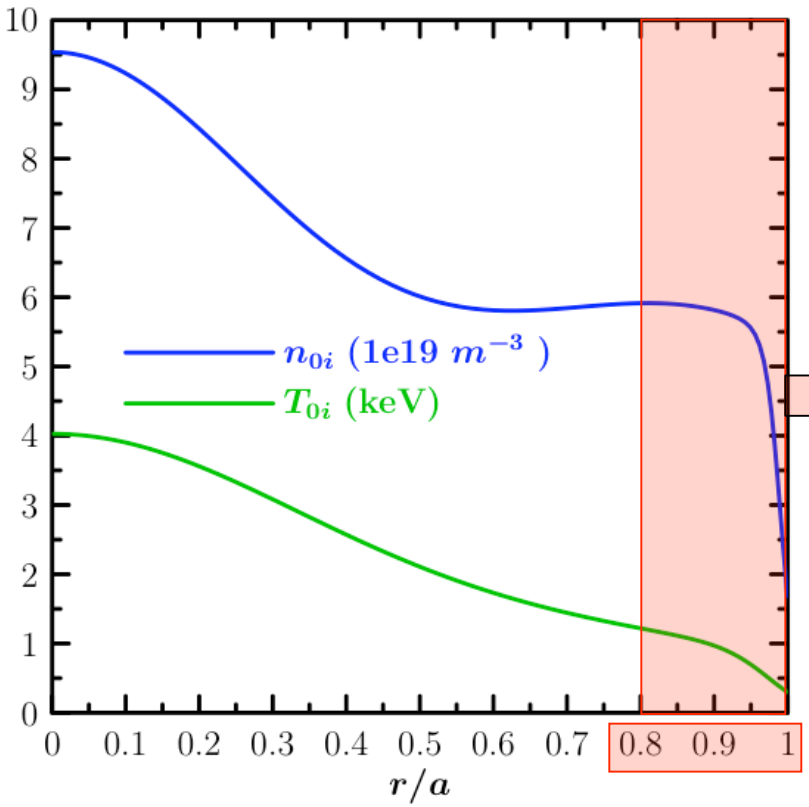
R_0=4 m, a=1m, q=3, B_0=4 T, $(n_{0i},T_{0i}) \sim c_1+c_2\exp(-c_3(r/a)^3)$, s-α geometry, adiabatic ele

GENERAL ATOMICS

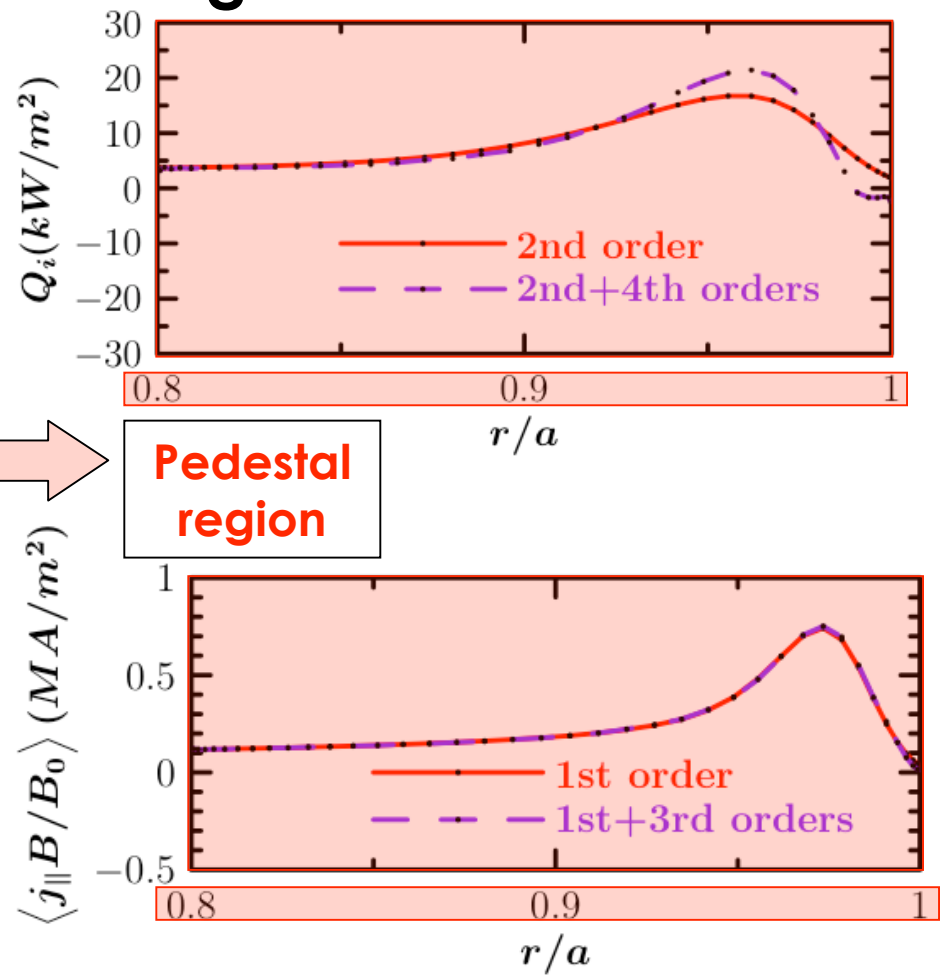
However, for typical DIII-D plasmas, only a weak FOW effect is found due to steep gradients in the H-mode edge.

DIII-D H-mode profiles

shot#132010, t=2.5-3.5s



Higher-order NEO results



DIII-D data provided by A. Leonard, T. Osborne, & R. Groebner.
Simulations done with s-a geometry.

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

- **Verification/analytic comparisons**
  - Agreement with Taguchi's theory for the full HS collision op.
  - CH theory overestimates Q_i for intermediate ε.
  - The Sauter model overestimates the bootstrap current.
- **Comparisons w/ NCLASS**
  - Corrections ~17% for the bootstrap current and ~30% for v_θ.
- **Impurity transport**
  - The HS multi-species theory gives a poor prediction of the ion and impurity fluxes.
- **Rotation effects**
  - Generally weak in typical experiments.
- **FOW effects**
  - Break-down of the δf formalism in the small region $r < r_{potato} \Rightarrow$ full F required.
  - Only a weak FOW effect in the DIII-D H-mode edge.

More details: E. Belli & J. Candy, PPCF 50, 095010 (2008).