

# Closure theory of partially ionized plasmas

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# General moment equations

- Landau (Fokker-Planck) kinetic equation

$$\frac{\partial f_a}{\partial t} + \mathbf{v} \cdot \nabla f_a + \frac{q_a}{m_a} (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \partial_{\mathbf{v}} f_a = \sum_b C(f_a, f_b)$$

- Moment expansion:  $m^{lk}$  is a symmetric traceless fluid moment

$$f_a(t, \mathbf{x}, \mathbf{v}) = f_a^M \sum_{lk} m_a^{lk}(t, \mathbf{x}) \cdot \hat{\mathbf{P}}^{lk}(\mathbf{c}_a)$$

$$n_a^{lk} \equiv n_a m_a^{lk}(t, \mathbf{x}) = \int d\mathbf{v} \hat{\mathbf{p}}_a^{lk} f_a(t, \mathbf{x}, \mathbf{v})$$

where  $\mathbf{c}_a = (\mathbf{v} - \mathbf{V}_a)/v_{Ta}$

- General moment equations [Ji Held 2006 2008 PoP]

$$\mathcal{L}_a \left[ \left( \frac{\partial}{\partial t}, \nabla \right) (T_a, \mathbf{V}_a), \mathbf{E} \right] n_a + \Omega_a \mathbf{b} \times n_a = \sum_b (A_{ab} n_a + B_{ab} n_b)$$

$(l, k) = (0,0)$  density ( $n$ ),  $(0,1)$  temperature ( $T$ ),  $(1,0)$  flow velocity ( $\mathbf{V}$ )  
 $(1,1)$  heat flow ( $\mathbf{h}$ ), and  $(2,0)$  viscosity tensor ( $\boldsymbol{\pi}$ )

# Fluid equations and closures/transport

Maxwellian moment  $(n_a, \mathbf{V}_a, T_a)$  equations

$$(0,0) \quad d_t n_a + n_a \nabla \cdot \mathbf{V}_a = 0 \quad (d_t \equiv \partial_t + \mathbf{V}_a \cdot \nabla)$$

$$(0,1) \quad \frac{3}{2} n_a d_t T_a + n_a T_a \nabla \cdot \mathbf{V}_a + \nabla \cdot \mathbf{h}_a + \nabla \mathbf{V}_a : \boldsymbol{\pi}_a = Q_a$$

$$(1,0) \quad m_a n_a d_t \mathbf{V}_a - n_a q_a (\mathbf{E} + \mathbf{V}_a \times \mathbf{B}) + \nabla p_a + \nabla \cdot \boldsymbol{\pi}_a = \mathbf{R}_a$$

$$(1,1) \quad d_t \mathbf{h} + \Omega \mathbf{b} \times \mathbf{h} + \frac{7}{5} (\nabla \cdot \mathbf{V}) \mathbf{h} + \frac{7}{5} \mathbf{h} \cdot (\nabla \mathbf{V}) + \frac{2}{5} (\nabla \mathbf{V}) \cdot \mathbf{h} + \frac{5p}{2m} \nabla T \\ + \frac{T}{m} \nabla \cdot \boldsymbol{\pi} + \frac{7}{2} \frac{\nabla T}{m} \cdot \boldsymbol{\pi} - \mathbf{a} \cdot \boldsymbol{\pi} + \nabla \cdot \boldsymbol{\theta} + \frac{1}{3} \nabla u^{02} + \nabla \mathbf{V} : u^{30} \\ = C_{10}^1 \mathbf{V}_{ei} + C_{11}^1 \mathbf{h} + C_{12}^1 \mathbf{r} + \dots \quad (\mathbf{h} \text{ heat flow})$$

$$(1,2) \quad d_t \mathbf{r} + \Omega \mathbf{b} \times \mathbf{r} + \dots = C_{10}^1 \mathbf{V}_{ei} + C_{21}^1 \mathbf{h} + C_{22}^1 \mathbf{r} + \dots \quad (\mathbf{r} \text{ heat heat flow})$$

$$(2,0) \quad d_t \boldsymbol{\pi} + \Omega \mathbf{b} \times \boldsymbol{\pi} + (\nabla \cdot \mathbf{V}) \boldsymbol{\pi} + 2 \boldsymbol{\pi} \cdot (\nabla \mathbf{V}) + pW + \frac{4}{5} \nabla \overline{\mathbf{h}} + \nabla \cdot u^{30} \\ = C_{00}^2 \boldsymbol{\pi} + C_{01}^2 \boldsymbol{\theta} + \dots \quad (\boldsymbol{\pi} \text{ viscosity})$$

$$(2,1) \quad d_t \boldsymbol{\theta} + \Omega \mathbf{b} \times \boldsymbol{\theta} + \dots = C_{10}^2 \boldsymbol{\pi} + C_{11}^2 \boldsymbol{\theta} + \dots \quad (\boldsymbol{\theta} \text{ heat viscosity})$$

$$\text{where } \mathbf{a} = \frac{q}{m} (\mathbf{E} + \mathbf{V} \times \mathbf{B}) - d_t \mathbf{V} \text{ and } W = \nabla \mathbf{V} + (\nabla \mathbf{V})^T - \frac{2}{3} \nabla \cdot \mathbf{V} \mathbf{I}$$

Closures: express  $\mathbf{h}_a(n_a^{11})$ ,  $\boldsymbol{\pi}_a(n_a^{20})$ ,  $Q_a$ ,  $\mathbf{R}_a$  in terms of  $n_a, \mathbf{V}_a, T_a$

Electron closures for high collisionality (Braginskii)

$$\mathbf{h}_e = (\beta)(\mathbf{V}_{ei}) - (\kappa_e)(\nabla T_e), \quad \mathbf{R}_e = -\mathbf{R}_i = -(\alpha)(\mathbf{V}_{ei}) - (\beta)(\nabla T_e)$$

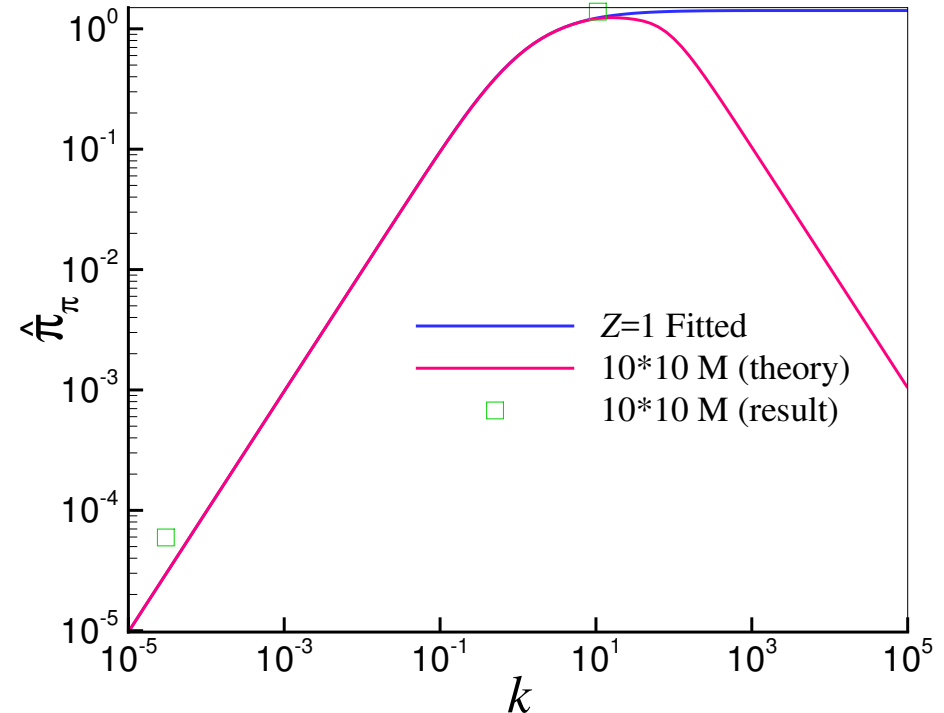
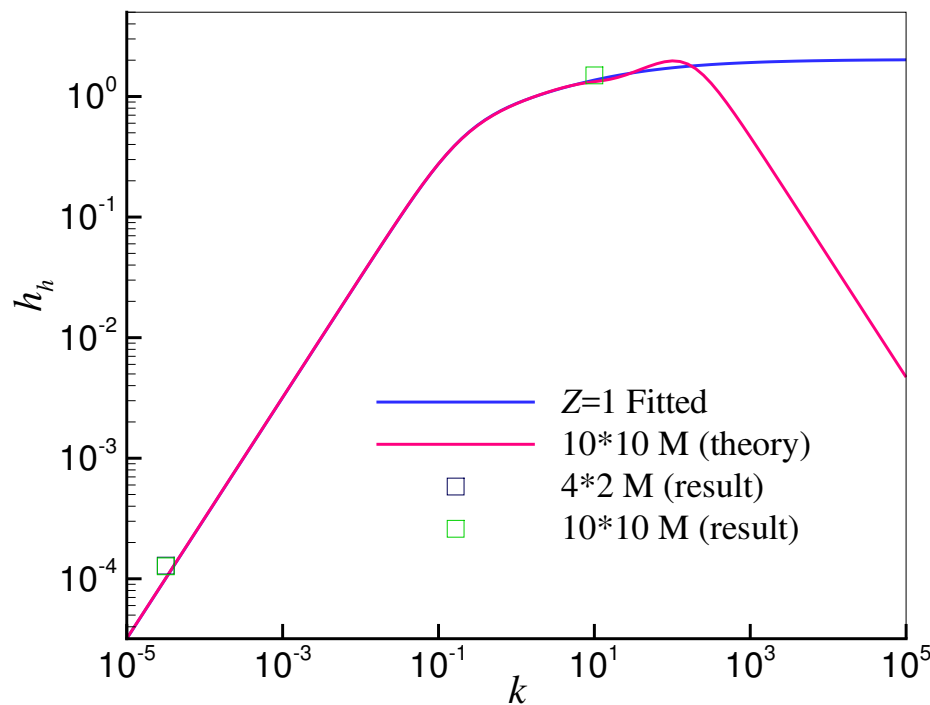
$$\mathbf{h}_i = -(\kappa_i)(\nabla T_i), \quad \boldsymbol{\pi}_e = -(\eta_e)(\nabla \mathbf{V}_e), \quad \boldsymbol{\pi}_i = -(\eta_i)(\nabla \mathbf{V}_i)$$

Transport: relate flux densities  $\mathbf{h}_e, \mathbf{J}$  to thermodynamic forces  $\nabla T_e$  and  $\mathbf{E}$

$$\mathbf{h}_e = (\tilde{\alpha}) \mathbf{E} - (\tilde{\kappa})(\nabla T_e), \quad \mathbf{J} = (\tilde{\sigma}) \mathbf{E} - (\tilde{\alpha})(\nabla T_e)$$

# Parallel moment equations in NIMROD

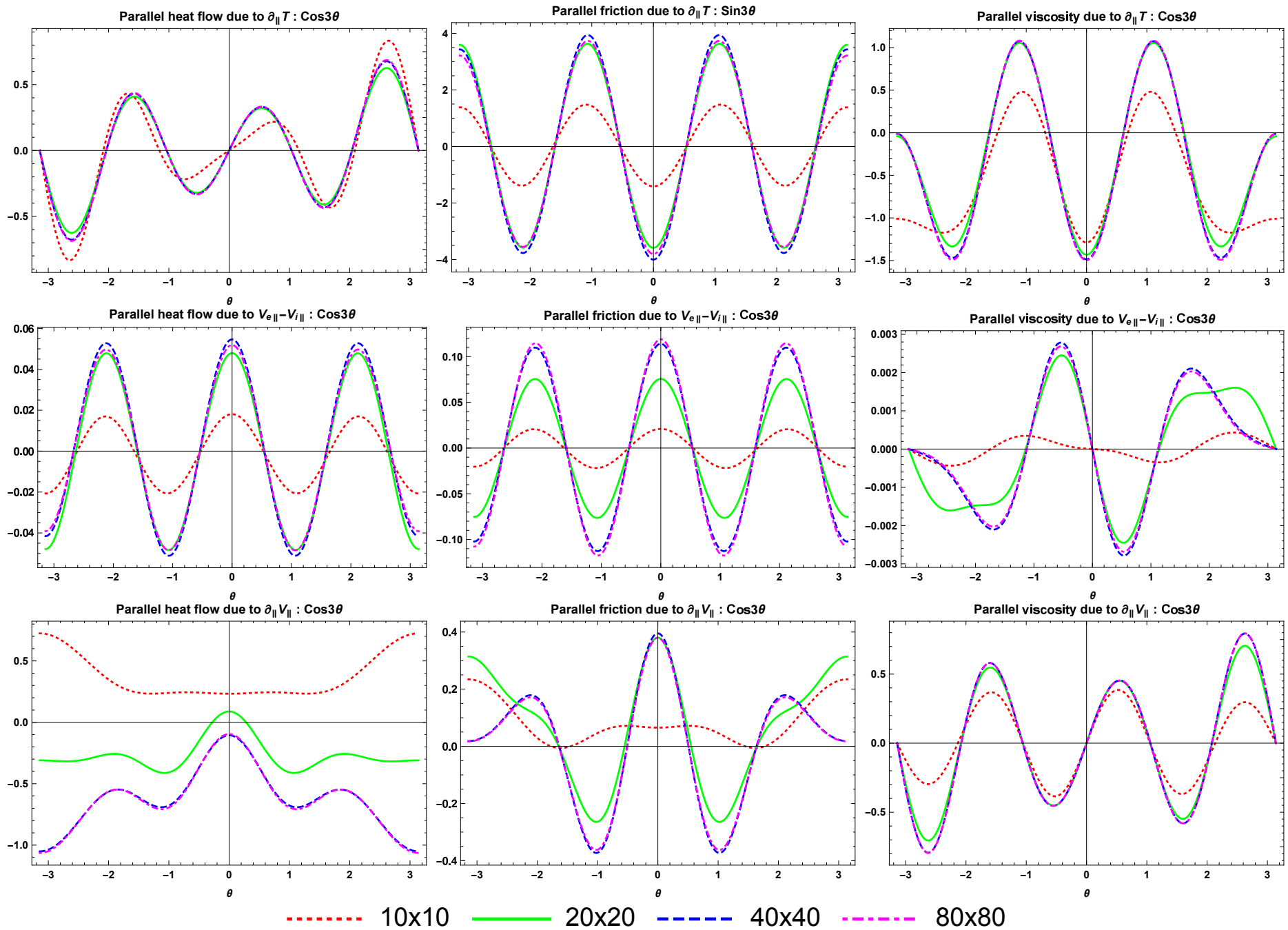
$$\frac{\partial}{\partial t} [n] + v_T \Psi \partial_{\parallel} [n] + \underbrace{v_T (\partial_{\parallel} \ln B) \Psi_B [n]}_{\text{inhomo. magnetic field}} + \underbrace{v_T (\partial_{\parallel} \ln T) \Phi [n] + \frac{q}{2T} E_{\parallel} \Theta [n]}_{\text{nonlinear coupling terms}} = \frac{1}{\tau} c [n] + [g]$$



Parallel heat flow and viscosity responding to the temperature and flow velocity gradients, respectively. The NIMROD results (squares) are compared to the analytical integral closures.

# Parallel closures in an inhomogeneous magnetic field

( $\epsilon = r/R = 0.5$ )



# Kinetic equations for a partially ionized plasma

$$\frac{\partial f_n}{\partial t} + \mathbf{v} \cdot \frac{\partial f_n}{\partial \mathbf{r}} + \frac{\mathbf{F}_n}{m_n} \cdot \frac{\partial f_n}{\partial \mathbf{v}} = X(f_n, f_i) + Y(f_i) - Z(f_n)$$

$$\frac{\partial f_i}{\partial t} + \mathbf{v} \cdot \frac{\partial f_i}{\partial \mathbf{r}} + \frac{\mathbf{F}_i}{m_i} \cdot \frac{\partial f_i}{\partial \mathbf{v}} = C(f_i) - X(f_n, f_i) - Y(f_i) + Z(f_n)$$

$$\frac{\partial f_e}{\partial t} + \mathbf{v} \cdot \frac{\partial f_e}{\partial \mathbf{r}} + \frac{\mathbf{F}_e}{m_e} \cdot \frac{\partial f_e}{\partial \mathbf{v}} = C(f_e) - Y(f_e, f_i) + Z(f_e, f_n)$$

$$\text{Recom: } Y(f_e, f_i) = \int d\mathbf{v}' \sigma_r |\mathbf{v} - \mathbf{v}'| f_i(\mathbf{v}') f_e(\mathbf{v})$$

$$Y(f_i) = Y(f_i, f_e) = \int d\mathbf{v}' \sigma_r |\mathbf{v} - \mathbf{v}'| f_e(\mathbf{v}') f_i(\mathbf{v}) \approx n_e \langle \sigma_r v_e \rangle f_i(\mathbf{v})$$

$$\text{Ioniz: } Z(f_e, f_n) = \int d\mathbf{v}' \sigma_z |\mathbf{v} - \mathbf{v}'| [f_e(\mathbf{v}_f) f_i(\mathbf{v}') - f_e(\mathbf{v}) f_n(\mathbf{v}')] + \frac{\delta f_e^{\text{created}}(\mathbf{v})}{\delta t}$$

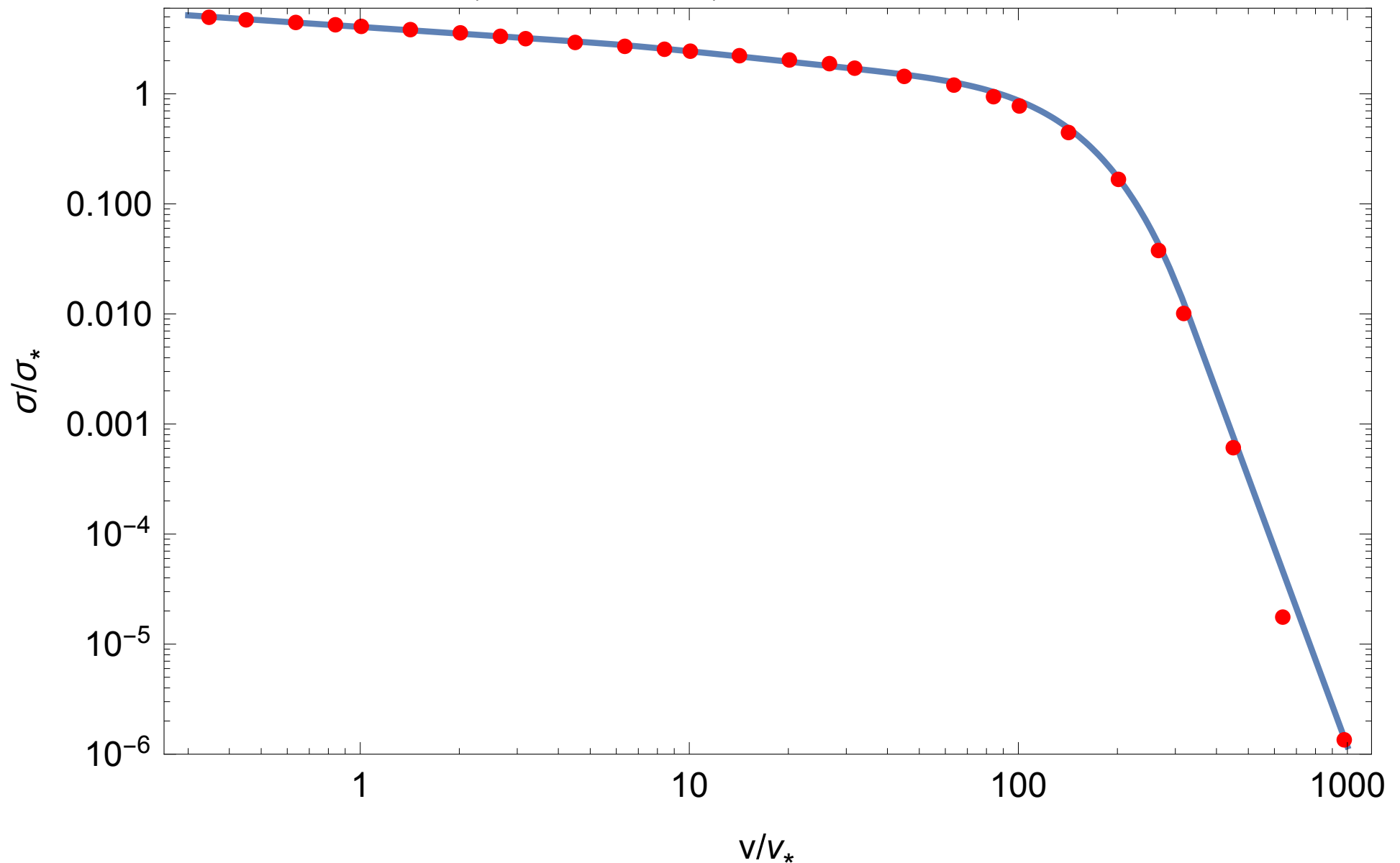
$$Z(f_n) = Z(f_n, f_e) = \int d\mathbf{v}' \sigma_z |\mathbf{v} - \mathbf{v}'| f_e(\mathbf{v}') f_n(\mathbf{v}) \approx n_e \langle \sigma_z v_e \rangle f_n(\mathbf{v})$$

$$\text{McWhirter 1965 } \langle \sigma_r v_e \rangle = 7.57 \times 10^{-18} \sqrt{\frac{13.6\text{eV}}{T_e}} \text{ m}^3/\text{s (not } 0.7 \times 10^{-19})$$

$$\text{Voronov 1997 } \langle \sigma_z v_e \rangle = 2.91 \times 10^{-14} \frac{(13.6\text{eV}/T_e)^{0.39}}{0.232 + 13.6\text{eV}/T_e} \exp\left(-\frac{13.6\text{eV}}{T_e}\right) \text{ m}^3/\text{s}$$

# Cross section for the charge exchange operator

Atomic data for fusion vol. 1, C. F. Barnett, ORNL 1990



$$v_* = 1.38 \times 10^4 \text{ m/s and } \sigma_* = 10^{-19} \text{ m}^2$$

# Moments of the charge exchange operator $(a, b) = (n, i)$ or $(i, n)$

$$X(f_a, f_b) = \int d\mathbf{v}' \sigma_X |\mathbf{v} - \mathbf{v}'| [f_a(\mathbf{v}') f_b(\mathbf{v}) - f_a(\mathbf{v}) f_b(\mathbf{v}')] ]$$

$$\hat{A}_{ab}^{lpk} \mathbf{N}_a^{lk} = \int d\mathbf{v} \hat{\mathbf{P}}_a^{lp} X(f_a^0 \hat{\mathbf{P}}_a^{lk} \cdot \mathbf{M}_a^{lk}, f_b^0)$$

$$\hat{B}_{ab}^{lpk} \mathbf{N}_b^{lk} = \int d\mathbf{v} \hat{\mathbf{P}}_a^{lp} X(f_a^0, f_b^0 \hat{\mathbf{P}}_b^{lk} \cdot \mathbf{M}_b^{lk})$$

$$\int d\mathbf{v}' \sigma_X |\mathbf{v} - \mathbf{v}'| f_b^{lk}(\mathbf{v}') = n_b \sigma_* \mathbf{P}^l(\hat{\mathbf{v}}) \cdot \mathbf{M}_b^{lk} S_{ab}^{lk}, \quad \hat{w}_a = \frac{\frac{1}{2} m_a v^2}{T_a} = s_a^2$$

$$S_{ab}^{lk} = \frac{1}{\pi^{1/2}} \underbrace{\int_0^\infty d\hat{w}' \hat{w}'^{(l+1)/2} L_k^l(\hat{w}') e^{-\hat{w}'}}_{\text{Gauss-Laguerre}} \underbrace{\int_{-1}^1 d\xi' P_l(\xi') \hat{\sigma}_X |\mathbf{v} - \mathbf{v}'|}_{\text{Gauss-Legendre}}$$

$$\begin{aligned} \sigma_l A_{ab}^{lpk} \mathbf{M}_a^{lk} &= - \int d\mathbf{v} \mathbf{P}_a^{lp}(\mathbf{s}_a) \int d\mathbf{v}' \sigma_X |\mathbf{v} - \mathbf{v}'| [f_a^{lk}(\mathbf{v}) f_b^0(\mathbf{v}') - f_a^{lk}(\mathbf{v}') f_b^0(\mathbf{v})] \\ &= -\sigma_l n_b \sigma_* \mathbf{N}_a^{lk} \frac{2}{\sqrt{\pi}} \int d\hat{w} \hat{w}^{(1+l)/2} L_p^l(\hat{w}) e^{-\hat{w}} \\ &\quad \times [\hat{w}^{l/2} L_k^l(\hat{w}) S_{ab}^{00} - S_{aa}^{lk} (T_b^a)^{3/2} e^{\hat{w}(1-T_b^a)}] \end{aligned}$$

$$\begin{aligned} \sigma_l B_{ab}^{lpk} \mathbf{M}_a^{lk} &= - \int d\mathbf{v} \mathbf{P}_a^{lp}(\mathbf{s}_a) \int d\mathbf{v}' \sigma_X |\mathbf{v} - \mathbf{v}'| [f_a^0(\mathbf{v}) f_b^{lk}(\mathbf{v}') - f_a^0(\mathbf{v}') f_b^{lk}(\mathbf{v})] \\ &= -\sigma_l n_a \sigma_* \mathbf{N}_b^{lk} \frac{2}{\sqrt{\pi}} \int d\hat{w} \hat{w}^{(1+l)/2} L_p^l(\hat{w}) e^{-\hat{w}} \end{aligned}$$



# Ion closures: kinetic equation

- Sum of neutral and ion equations

$$\frac{\partial f_i}{\partial t} + \mathbf{v} \cdot \frac{\partial f_i}{\partial \mathbf{r}} + \mathbf{a}_i \cdot \frac{\partial f_i}{\partial \mathbf{v}} + \frac{\partial f_n}{\partial t} + \mathbf{v} \cdot \frac{\partial f_n}{\partial \mathbf{r}} + \mathbf{a}_n \cdot \frac{\partial f_n}{\partial \mathbf{v}} = C(f_i)$$

- Set  $f = f^M + f^N$

Solve the kinetic equation to express  $f^N$  in terms of  $f^M$

Take closure moments to express **closures** in terms of **thermodynamic drives**

- Asymptotic closure scheme

Adopt the closure ordering:  $\frac{\partial f^N}{\partial t} = 0$

Ignore  $\mathbf{v} \cdot \frac{\partial f^N}{\partial \mathbf{r}}$  and  $\frac{q}{m} \mathbf{E} \cdot \frac{\partial f^N}{\partial \mathbf{v}} \Leftarrow$  only for high collisionality

$$\mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} (f_i^M + f_n^M) - \frac{q_i}{m_i} \mathbf{v} \times \mathbf{B} \cdot \frac{\partial f_i^N}{\partial \mathbf{v}} = C(f_i^M, f_e^M) + C_{iL}(f_i^N) + \text{Maxwellian}$$

# Ion closures: moment equations

- Take moments of  $C_{iL}(f_i^N) - \frac{q_i}{m_i} \mathbf{v} \times \mathbf{B} \cdot \frac{\partial f_i}{\partial \mathbf{v}} = -\mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} (f_i^M + f_n^M) + C(f_i^M, f_e^M)$

$$-C_i^l N_i^l + \Omega_i \mathbf{b} \times N_i^l = G_i^{\nabla, l} + G_n^{\nabla, l} \Rightarrow \nabla(T_i + T_n) \text{ and } W_i + W_n$$

$$l = 1 : -\frac{1}{\tau_{ii}} c_i N_i^1 + \Omega_i \mathbf{b} \times N_i^1 = g^1 \left( \frac{n_i v_{Ti}}{T_i} \nabla T_i + \frac{n_n v_{Tn}}{T_n} g^1 \nabla T_n \right), \quad g^1 \equiv \begin{pmatrix} \frac{\sqrt{5}}{2} \\ 0 \\ \vdots \end{pmatrix}$$

- General solution of a set of vector equations

Define  $\mathbf{g}_{\parallel} \equiv \mathbf{b} \mathbf{b} \cdot \mathbf{g}$ ,  $\mathbf{g}_{\times} \equiv \mathbf{b} \times \mathbf{g}$ ,  $\mathbf{g}_{\perp} \equiv -\mathbf{b} \times (\mathbf{b} \times \mathbf{g})$

$$-c\mathbf{N} + r\mathbf{b} \times \mathbf{N} = \mathbf{g} \Rightarrow \mathbf{N} = - \left[ c^{-1} \mathbf{g}_{\parallel} + \frac{1}{c^2 + r^2} (r\mathbf{g}_{\times} + c\mathbf{g}_{\perp}) \right]$$

$$N_{i,a}^1 = -\frac{n_a v_{Ta} \tau_{ii}}{T_a} [\mathbf{i} g_{\parallel} \nabla_{\parallel} T_a + \mathbf{i} g_{\times} \nabla_{\times} T_a + \mathbf{i} g_{\perp} \nabla_{\perp} T_a]$$

$$N_i^1 = \begin{pmatrix} N_i^{11}(v^2 \mathbf{v}) \\ N_i^{12}(v^4 \mathbf{v}) \\ \vdots \end{pmatrix} = N_{i,i}^1 + N_{i,n}^1 \Rightarrow \mathbf{R}_{ni} \propto \sum_{k=1} \left( \hat{A}_{ni}^{10k} N_n^{1k} + \hat{B}_{ni}^{10k} N_i^{1k} \right) \quad \mathbf{h} = -\frac{\sqrt{5}}{2} T v_T N^{11}$$

# Neutral closures

$$\mathbf{v} \cdot \frac{\partial f_n^M}{\partial \mathbf{r}} = X(f_n^M, f_i^M) + X(f_n^N, f_i^M) + X(f_n^M, f_i^N) + Y(f_i^N) - Z(f_n^N)$$

Take moments:  $-\mathbf{G}_{\nabla, n}^l = \mathbf{G}_{X, n}^l + \mathbf{A}_{ni}^l \mathbf{N}_n^l + \mathbf{B}_{ni}^l \mathbf{N}_i^l + \mathbf{Y}_{ni}^l \mathbf{N}_i^l - \mathbf{Z}_{nn}^l \mathbf{N}_n^l$

$$\underbrace{\left( -a_{ni}^1 + \frac{\tau_X}{\tau_Z} z_{nn}^1 \right)}_{AZ} \mathbf{N}_n^1 = \frac{n_n v_{Tn} \tau_X}{T_n} \mathbf{g}^1 \nabla T_n + a_{ni}^{1.0} \frac{\sqrt{2} n_n \mathbf{V}_n}{v_{Tn}} + b_{ni}^{1.0} \frac{\sqrt{2} n_n \mathbf{V}_i}{v_{Ti}} + \left( b_{ni}^1 \frac{n_n}{n_i} + \frac{\tau_X}{\tau_Y} y_{ni}^1 \right) \mathbf{N}_i^1$$

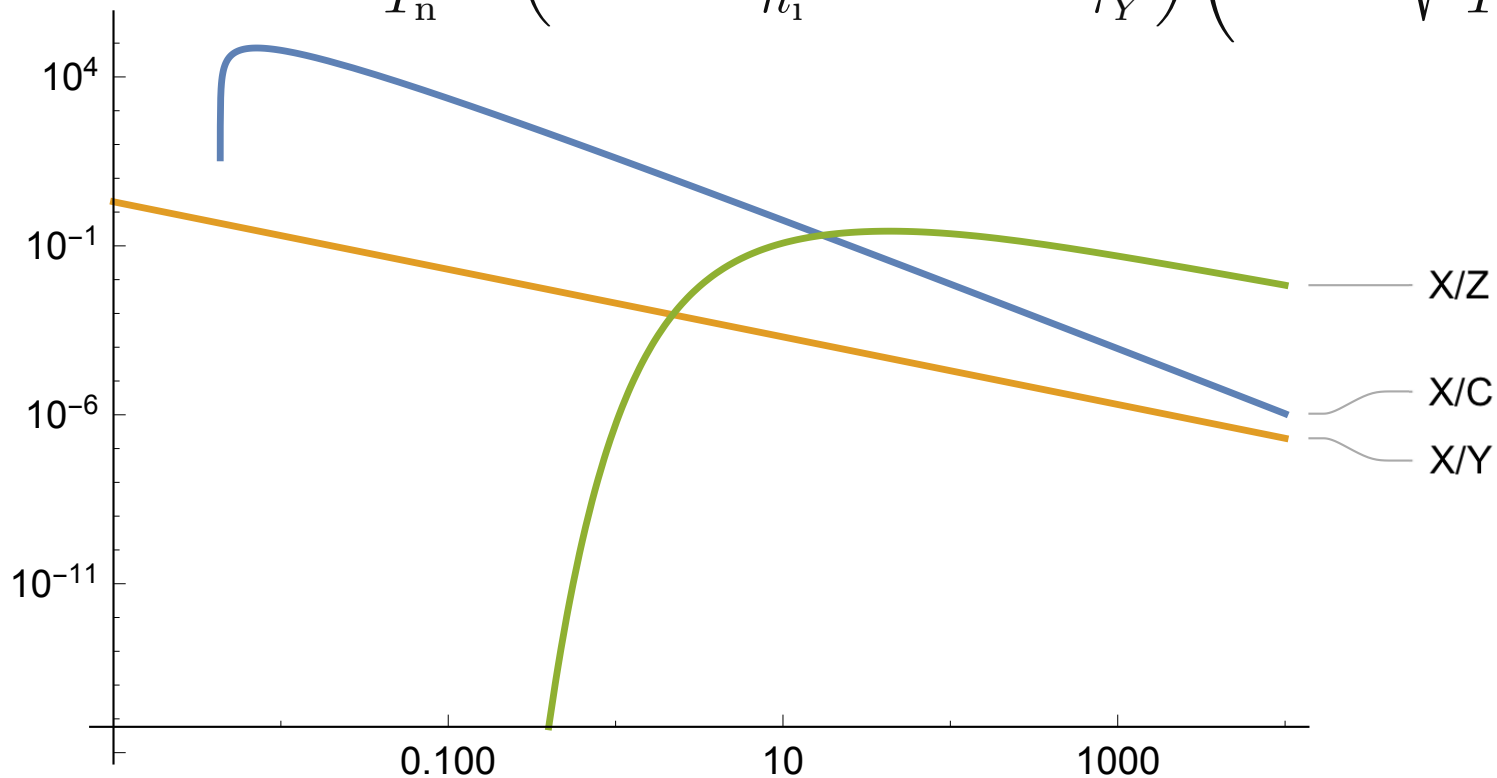
$$\begin{aligned} \mathbf{N}_n^1 = & \frac{n_n v_{Tn} \tau_X}{T_n} \left( \text{ngn} \nabla T_n + \text{nvn} \frac{\sqrt{2} n_n \mathbf{V}_n}{v_{Tn}} + \text{nvi} \frac{\sqrt{2} n_n \mathbf{V}_i}{v_{Ti}} \right) \\ & - \frac{n_n v_{Tn} \tau_{ii}}{T_n} \left( \text{ngl} \nabla_{\parallel} T_n + \text{ngx} \nabla_{\times} T_n + \text{ngp} \nabla_{\perp} T_n \right) \\ & - \frac{n_i v_{Ti} \tau_{ii}}{T_i} \left( \text{ngl} \nabla_{\parallel} T_i + \text{ngx} \nabla_{\times} T_i + \text{ngp} \nabla_{\perp} T_i \right) \end{aligned}$$

$$\mathbf{N}_n^1 = \frac{n_n v_{Tn} \tau_X}{T_n} \left( \text{ngn} \nabla_{\parallel} T_n + \text{nvn} \frac{\sqrt{2} n_n \mathbf{V}_{ni}}{v_{Tn}} \right) - \frac{n_n v_{Tn} \tau_{ii}}{T_n} \text{ngl} \left( \nabla_{\parallel} T_n + \sqrt{\frac{T_n}{T_i}} \frac{n_i}{n_n} \nabla_{\parallel} T_i \right) + \dots$$

where  $\text{ngl} = AZ^{-1} b_{ni}^1 \text{igl} \frac{n_n}{n_i} + AZ^{-1} y_{ni}^1 \text{igl} \frac{\tau_X}{\tau_Y} \equiv \text{nglbigl} \frac{n_n}{n_i} + \text{nglyigl} \frac{\tau_X}{\tau_Y}$

# Neutral closures (cont.)

$$N_n^1 = \frac{n_n v_{Tn} \tau_X}{T_n} \left( ngn \nabla_{\parallel} T_n + nvn \frac{\sqrt{2} n_n \mathbf{V}_{ni}}{v_{Tn}} \right) - \frac{n_n v_{Tn} \tau_{ii}}{T_n} \left( nglbig1 \frac{n_n}{n_i} + nglyig1 \frac{\tau_X}{\tau_Y} \right) \left( \nabla_{\parallel} T_n + \sqrt{\frac{T_n}{T_i}} \frac{n_i}{n_n} \nabla_{\parallel} T_i \right) + \dots$$



$T$ (eV)	0.03	1	10	100	1 k	10 k
$\tau_X / \tau_Y$	0.067	2.0E-3	2.0E-4	2.0E-5	2.0E-6	2.0E-7
$\tau_X / \tau_Z$	0	5.2E-7	0.12	0.23	0.050	0.0069
$\tau_X / \tau_{ii}$	1.6E4	40	0.57	0.0074	9.1E-5	1.1E-6

# Convergence with Gaussian nodes and moments ( $T = 100\text{eV}$ )

## Convergent results: heat flow vs. temperature

$$N_n^1 = \frac{n_n v_{Tn} \tau_X}{T_n} \left( ngn \nabla_{\parallel} T_n + nvn \frac{\sqrt{2} n_n \mathbf{V}_{ni}}{v_{Tn}} \right) - \frac{n_n v_{Tn} \tau_{ii}}{T_n} \left( nglbigl \frac{n_n}{n_i} + nglyigl \frac{\tau_X}{\tau_Y} \right) \dots$$

Gauss-Legendre nodes = 10 (or 20), ( $n_w$  = Gauss-Laguerre nodes), and moments M

ngn		(20)	(20)	nvn					
( $n_w = 10$ )	(20)	(40)	3M	4M	(10)	(20)	(40)	3M	4M
1.732	1.734	1.735	1.735	1.736	0.0689	0.0685	0.0684	0.0687	0.0687
0.174	0.173	0.172	0.179	0.180	0.0154	0.0150	0.0150	0.0156	0.0157
			0.049	0.052				0.0049	0.0049
				0.018					0.0018
nglbigl					nglyigl				
-1.371	-1.370	-1.369	-1.374	-1.375	-3.133	-3.137	-3.139	-3.140	-3.141
0.508	0.508	0.507	0.543	0.542	0.633	0.634	0.635	0.697	0.696
			-0.060	-0.043				-0.078	-0.054
				-0.021					-0.046

Heat flow results (3 vector moment approximation)

$T$ (eV)	0.03	1	10	100	1 k	10 k
ngn	1.05	1.50	1.59	1.73	3.81	34.7
nvn	0.127	0.127	0.0968	0.0685	0.0391	-0.305
nglbigl	-2.09	-2.09	-1.75	-1.37	-1.74	-1.57
nglyigl	-1.85	-2.63	-2.84	-3.14	-7.01	-76.8

# Future work

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- Closure coefficients for high collisionality

- ◇ Number of parameters

$$n_i, n_n, T_i, T_n \Rightarrow T_i, T_n$$

- ◇ Obtain functions of  $T_i$  and  $T_n$  fitted to closure coefficients

- Low collisionality

- ◇ Combine with collisionless-limit closures

Thanks!

Enjoy Moments and

Team Building Exercise!  
(the NIMROD open)