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Title: The physics of how a minority runaway electron population can dominate the charge state balance and radiative cooling of a post thermal quench plasma

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The physics of how a minority runaway electron population can dominate the charge state balance and radiative cooling of a post thermal quench plasma

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62nd Annual Meeting of the APS Division of Plasma Physics

With thanks…

A broad group working on improving how atomic data can help modeling fusion plasmas

LANL & TDS

- Xianzhu Tang
- Chris McDevitt (U. Florida)
- Jun Li
- Qi Tang
- Yanzeng Zhang

FLYCHK

- Hyun-Kyung Chung (NFRI, Korea)

A&M physics

- Chris Fontes
- Mark Zammit
- James Colgan

UQ & ML

- Tim Wildey (Sandia)
- Romit Maulik (Argonne)
- Prasanna Balaprakash (Argonne)

Students

- Todd Elder (Columbia)
- Yuzhi Li (VT)
- Andrew George (U. Houston)
- William Kupets (St John's Santa Fe)

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- DoE through OFES and the Tokamak Disruption Studies SciDAC
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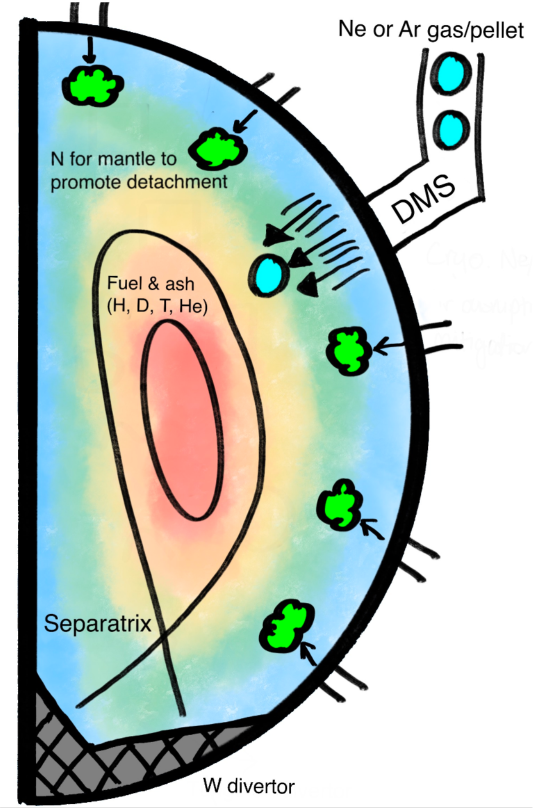
Goal of this talk

- Motivate a need to look closer at how to model RE and impurity interaction
- Outline some of the atomic physics that we need to take into account
- Some examples of how improved atomic physics data impacts disruption relevant discharges with minority RE

Motivation

Motivation: Impurities are vital for intended ITER operation



- Neon/argon for disruption mitigation
- Nitrogen for steady-state operation
- Be/W sputtering is inevitable
- Whatever the future of ITER brings…

When these impurities are present we want to know:

- Charge state population, ***n***
- Z_{eff}
- Radiative power loss, *RPL(**n**)*
- (As much as we can…)

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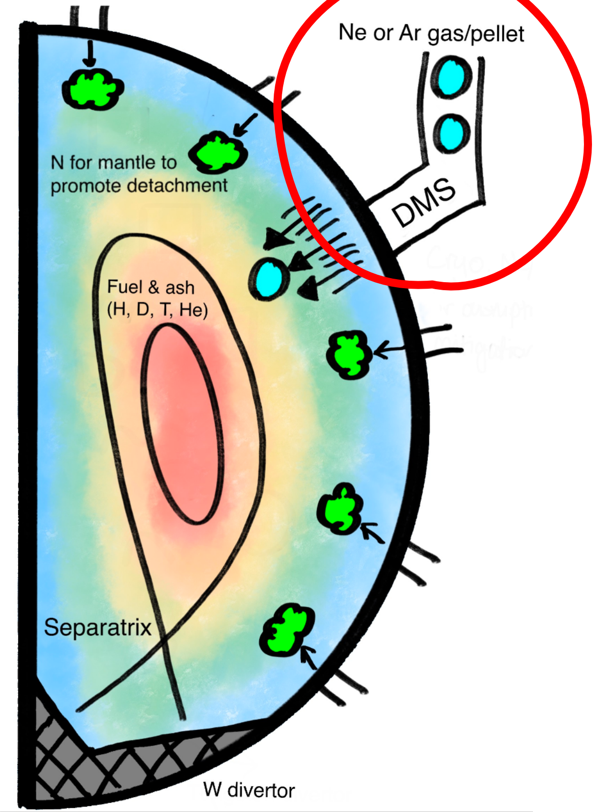

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How to model these quantities?

Charge state population, ***n***

Z_{eff}

Radiative power loss, *RPL(**n**)*

→ **Collisional-Radiative modeling**

$$\frac{d\mathbf{n}}{dt} = \mathrm{R}(\mathbf{n})\mathbf{n}$$

Assumptions:

Optically thin (tokamak, generally assumed low enough n_e)

Through this talk we focus on steady-state (LHS=0) – reasonable for RE plateau

Two atomic species defined by n_X and n_D densities

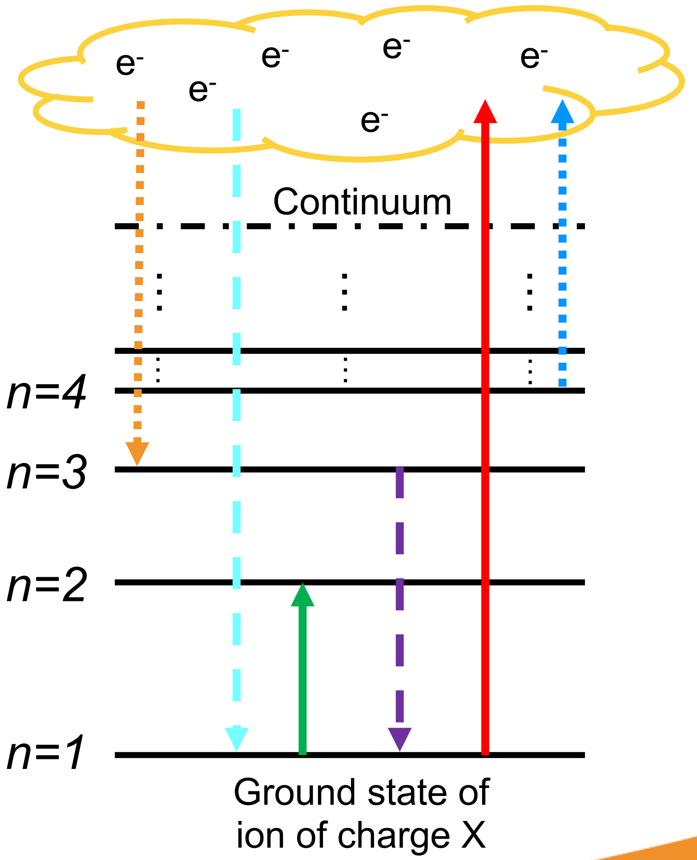
CR modeling

- State vector, ***n***, of excited states of each possible ion charge state

$$\mathrm{R}(\mathbf{n})\mathbf{n} = 0 \qquad \boldsymbol{n} = \begin{bmatrix} n_{Z,1} \\ n_{Z,2} \\ n_{Z,3} \\ n_{Z,4} \\ \ldots \end{bmatrix}$$

- Transitions between states populate rate matrix elements, $R_{i,i+1}$, describing excitation and ionization collisions, radiative decays, radiative recombination, autoionization & electron capture

$$R_{i,i+1} = n_e \int_{\Delta E}^{\infty} v f(E) \sigma_{i,i+1} dE$$



CR models in the fusion community

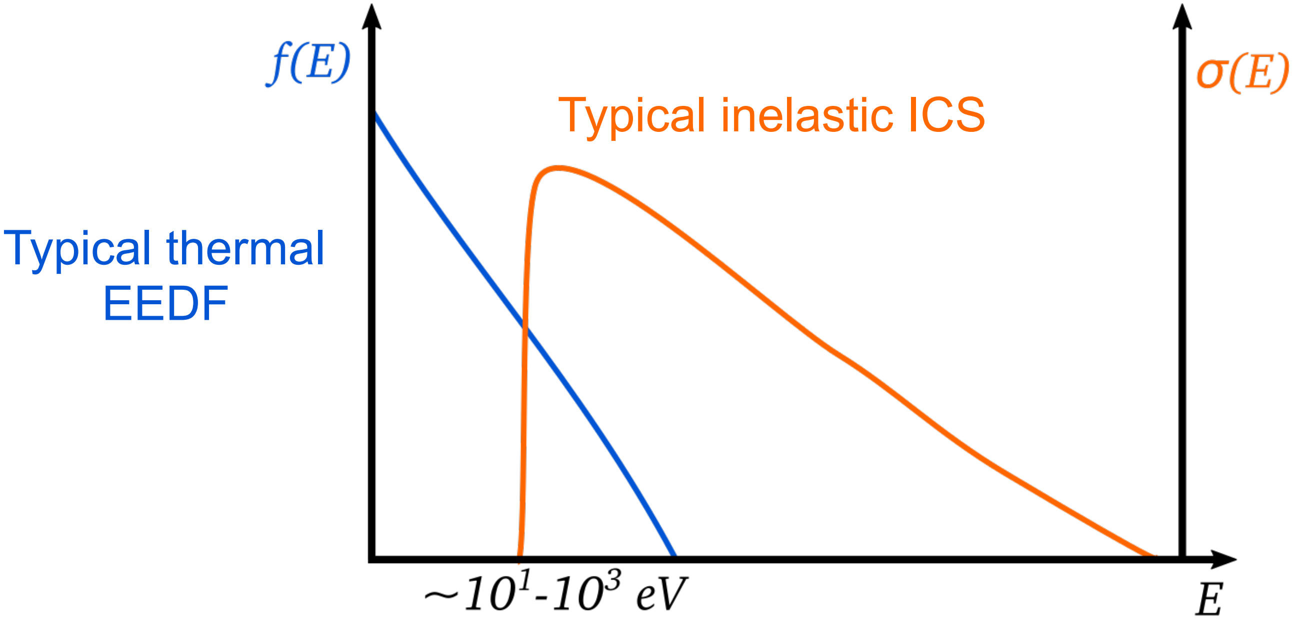
- US groups have long used KPRAD to couple with plasma codes and probe experiments on DIII-D, C-MOD [Whyte *et al.* Proceedings of the 24th European Conference on Controlled Fusion and Plasma Physics 21A:1137 (1997)]
- EU groups have used ADAS at a mature level [Summers *et al.* AIP Conference Proceedings 901, no. 1 (2007)]
- HEDP often uses FLYCHK [Chung *et al.* HEDP 1 3 (2005)]

General idea of this work:

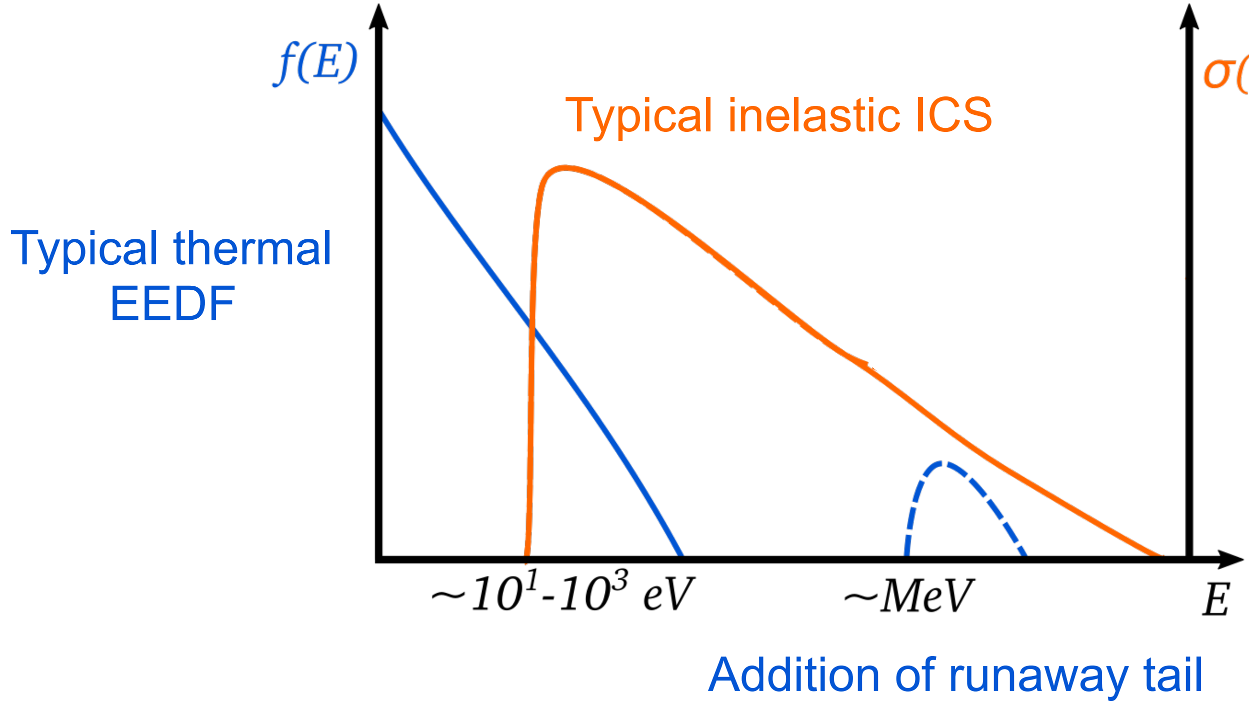
Do we need to do anything different from standard modeling to describe impact of runaways, and does it make a difference?

Relativistic electron impact scattering

Interaction of EEDF with inelastic cross-sections



Interaction of EEDF with inelastic cross-sections



Relativistic inelastic scattering

- Non-relativistic e^- - e^- scattering well served by Coulomb interaction
- Near light speed, e^- experience additional sizeable interactions

Breit interaction

e^- - e^- interaction = Coulomb interaction + magnetic correction + retarded correction

Repulsive electric potential

$\mu \cdot \mathbf{B}$

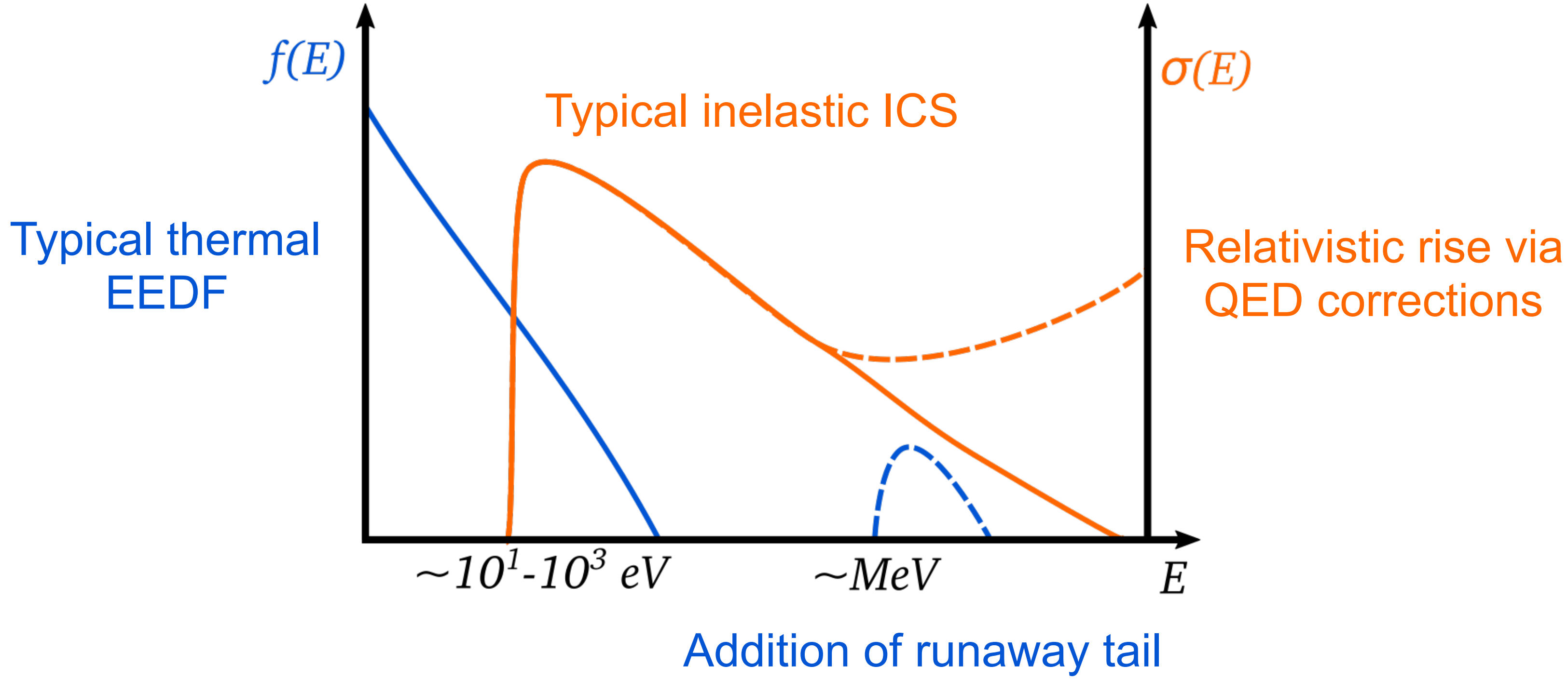
O(v_1 v_2 /c^2)

Finite c, delayed signal of electric force

Møller interaction

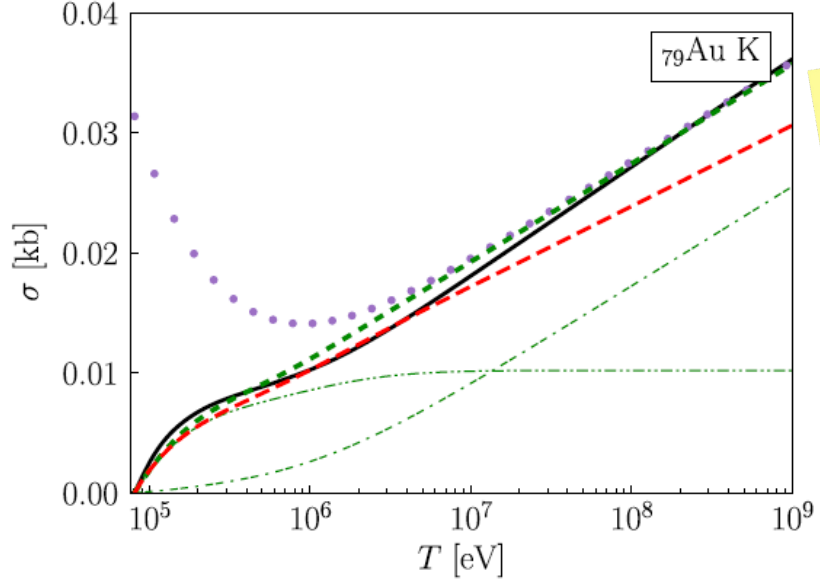
- QED formulations of generalized Breit or Møller interaction [Fontes *et al.* PRA **47** 2 (1993)]
- Historically employed for binding energy calculations and collisions under 'thermal' plasma conditions but not for collisions in ultra-relativistic limit

Interaction of EEDF with inelastic cross-sections



Sidebar: Even higher Z targets

- For higher Z targets, the relativistic enhancement can be the dominant part of inelastic scattering
- Example: K shell Gold Z=79 [Wang *et al.* J. Phys. B 51 145201 (2018)]



Gold Z=79 is close to Tungsten Z=74...

Our CR approach

- Developing fork of superconfiguration (n only) FLYCHK CR, flychklite, to allow relativistic corrections, scaled near-neutral cross sections, arbitrary EEDF. Retain excited states.
- Modify base excitation and ionization ICS in FLYCHK to transition to a relativistic ICS, also use BEB scaling* for NR cross sections of neutral and singly-ionized targets

$$\sigma_{i\to j}^{\mathrm{TOT}} = (1 - S(E))\sigma_{i\to j}^{\mathrm{NR}} + S(E)\sigma_{i\to j}^{\mathrm{R}}$$

- Simulate relativistic effect via Møller-Bethe-like analytic relativistic-rise

$$\sigma_I^{rel} \sim \left(\log\left(\frac{\beta^2}{1-\beta^2}\frac{0.5 m_e c^2}{\Delta I_Z^i}\right) - \beta^2\right) \qquad \beta = v/c$$

*YKK scaling - Yong-Ki Kim PRA 64 032713 (2001), PRA 65 022705 (2002)

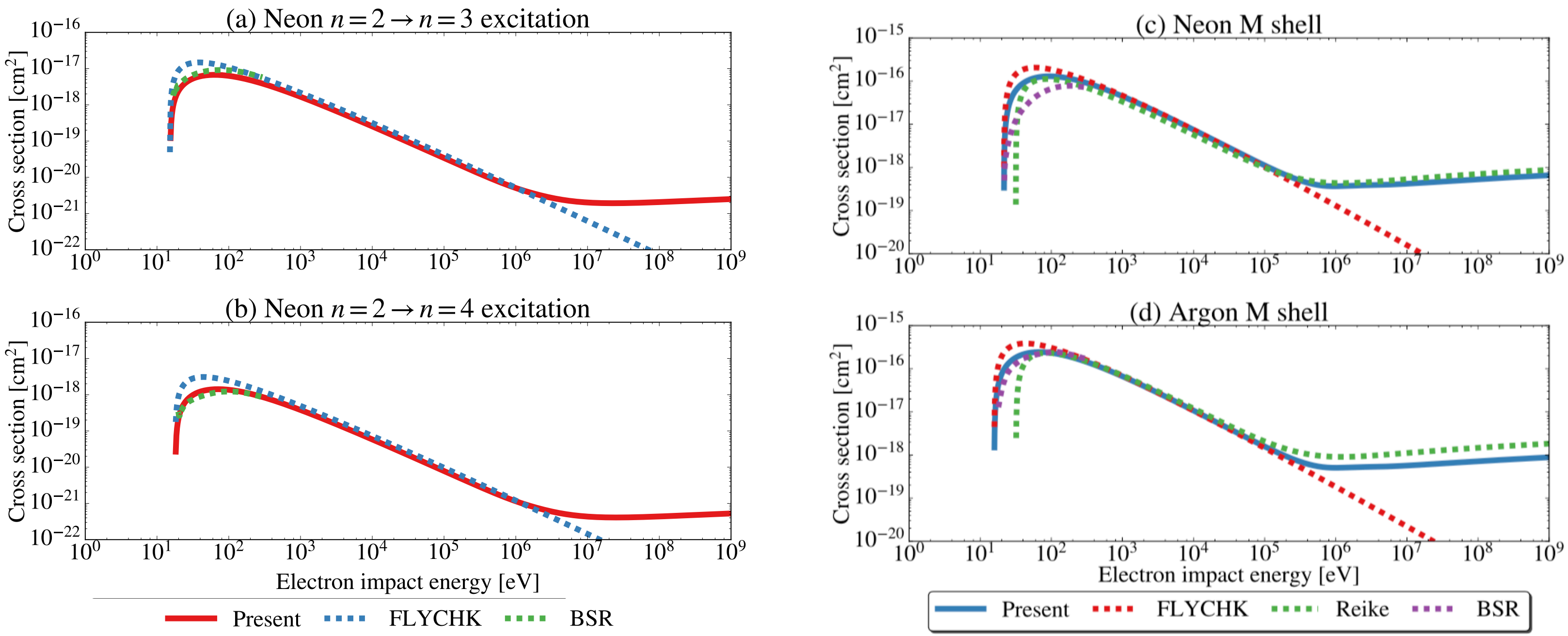
Modeling relativistic effect via Møller-Bethe-like analytic form

- Møller-Bethe-like form not a new thing

- Back to stopping power work of 1930s
  - Moller *Annalen der Physik* 406 5 (1932)
  - Bethe *Z. Physik* 76 5 (1932)
  - Recently Hollmann *et al.* Nucl. Fusion 59 106014 (2019)

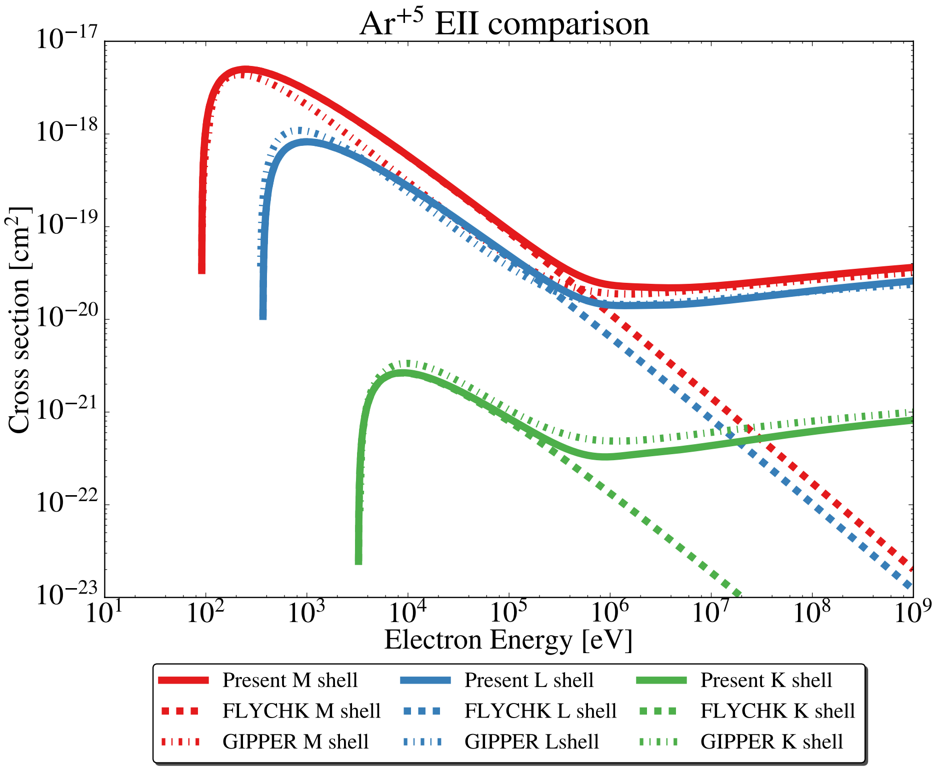
- Provides a general prescription we can apply to any inelastic collision
  - But we try to benchmark and tune general formulas against QM calculations that are available

Example cross section benchmarking



BSR – B-Spline R matrix calculations of Zatsarinny & Bartschat available online at www.lxcat.net
Reike – Reike & Prepejchal PRA 6 4 (1972)

Example cross section benchmarking



How does this relativistic correction change things?

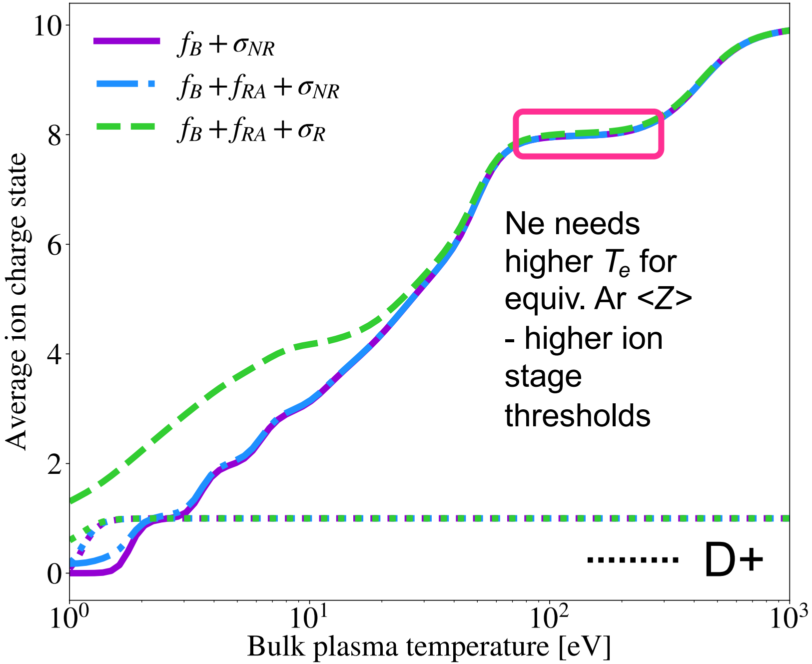
A simple comparison

- Lets compare effect of RE tail plus relativistic ICS
- Vary bulk thermal T_e
- Simplest f(E) assumption – Maxwellian or Bi-Maxwellian
  - T_{tail} = 10 MeV – gives RE tail peak at approx. 5 MeV
  - Fixed ion densities: n_D=n_{Ar} or n_D=n_{Ne} = 1x10^{20} m^{-3}
  - Fixed n_{RA} = 5x10^{16} m^{-3} - roughly a 5MA ITER-like RE current

- Let's compare for neon and argon with varying f(E) and cross sections:
  - base thermal case
  - with RE tail but NR cross sections
  - with RE tail and relativistic corrections

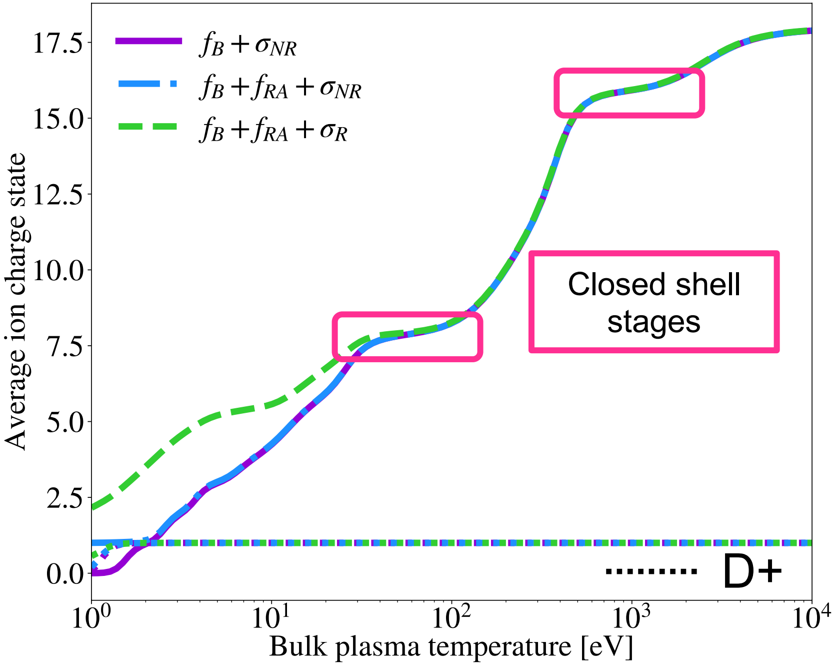
<Z> for this comparison

n_D=n_{Ne} =1x10[20] m[-3] , n_{RA} = 5x10[16] m[-3]



Neon

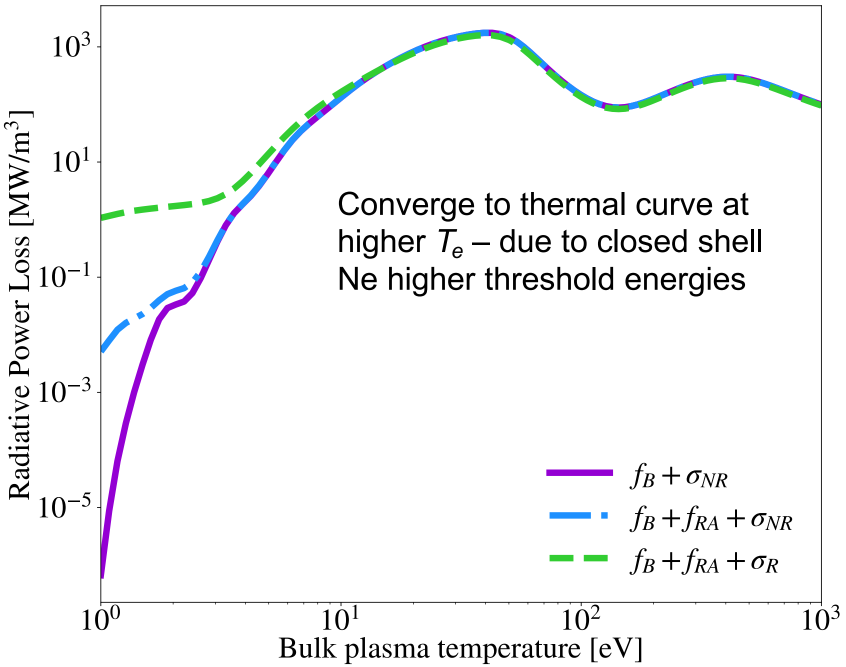
n_D=n_{Ar} =1x10[20] m[-3] , n_{RA} = 5x10[16] m[-3]



Argon

RPL for this comparison – line emission

n_D=n_{Ne} =1x10^{20} m^{-3} , n_{RA} = 5x10^{16} m^{-3}



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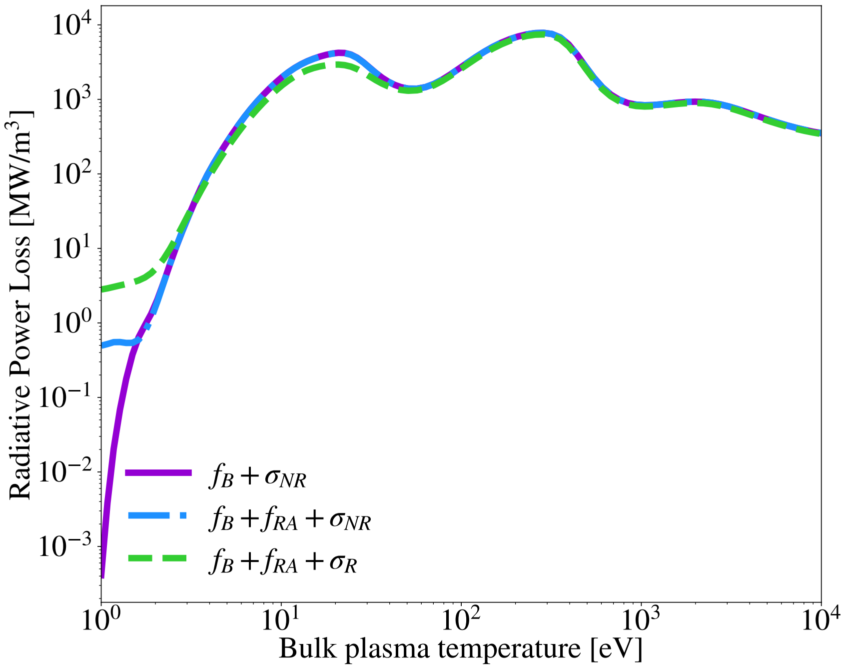
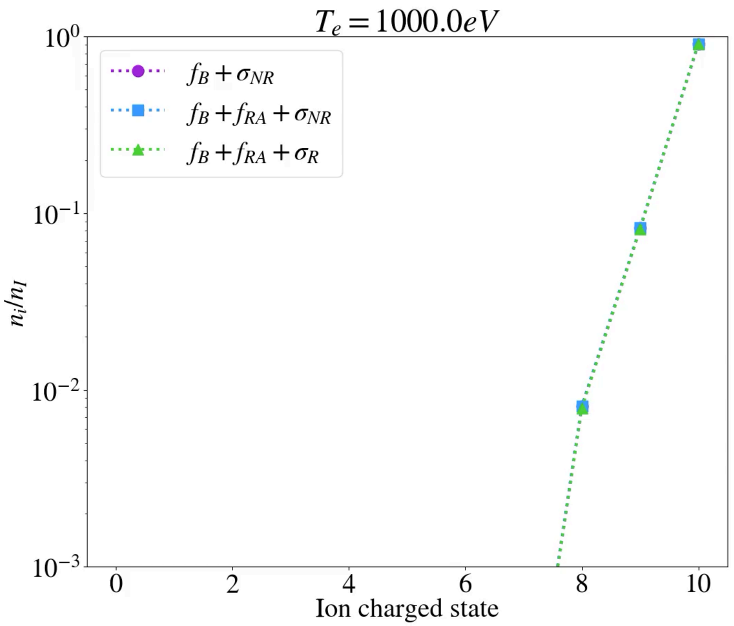
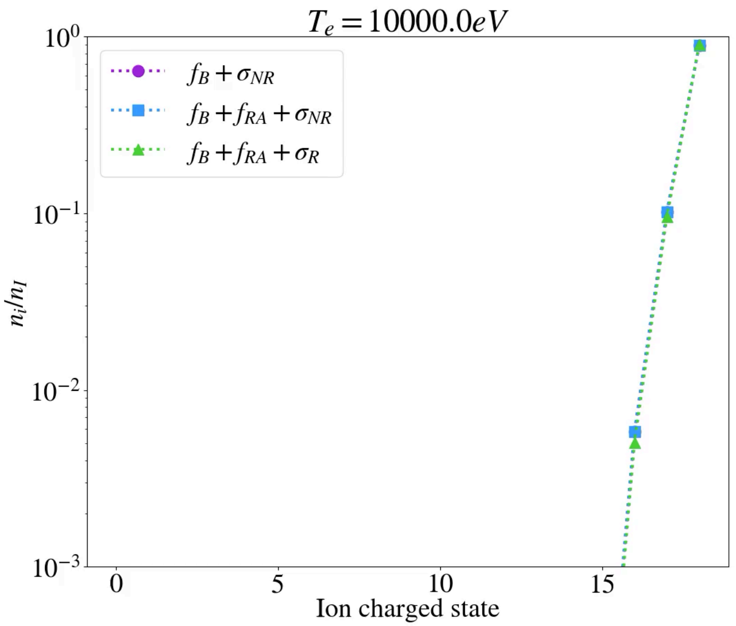


Argon

CSD with reducing T_e



Neon



Argon

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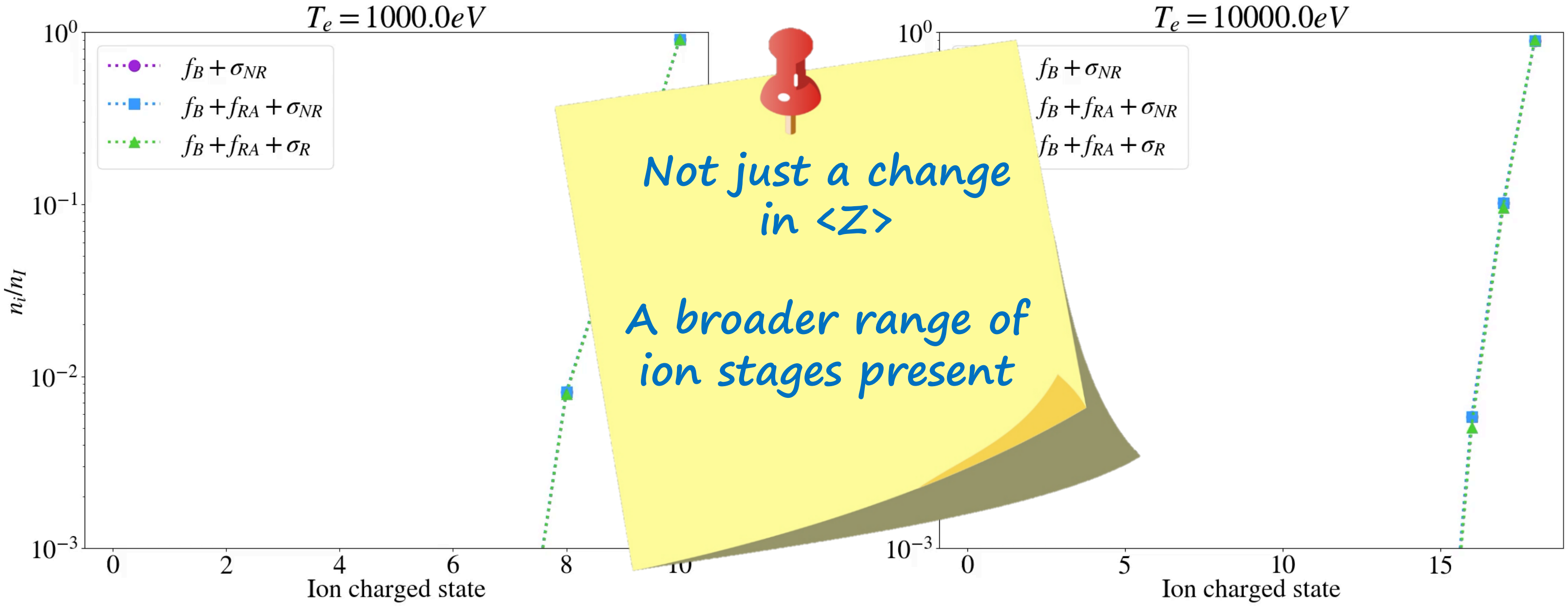
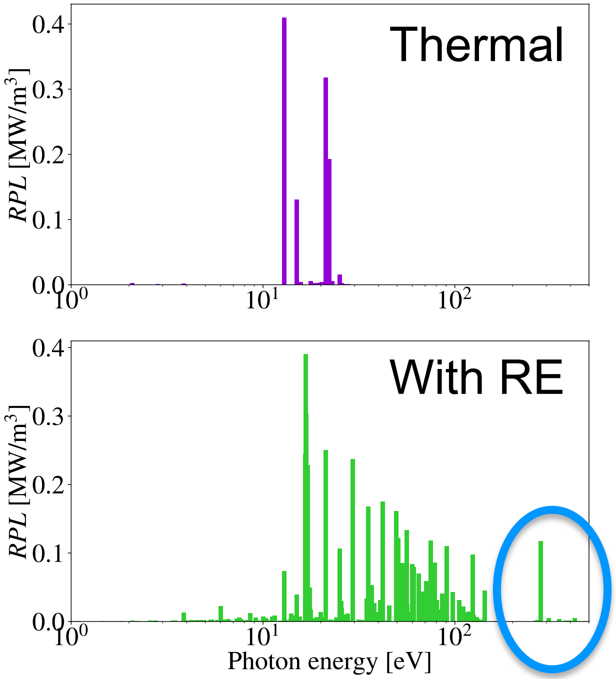


Neon

Argon

Clear spectral differences

T_e = 2 eV

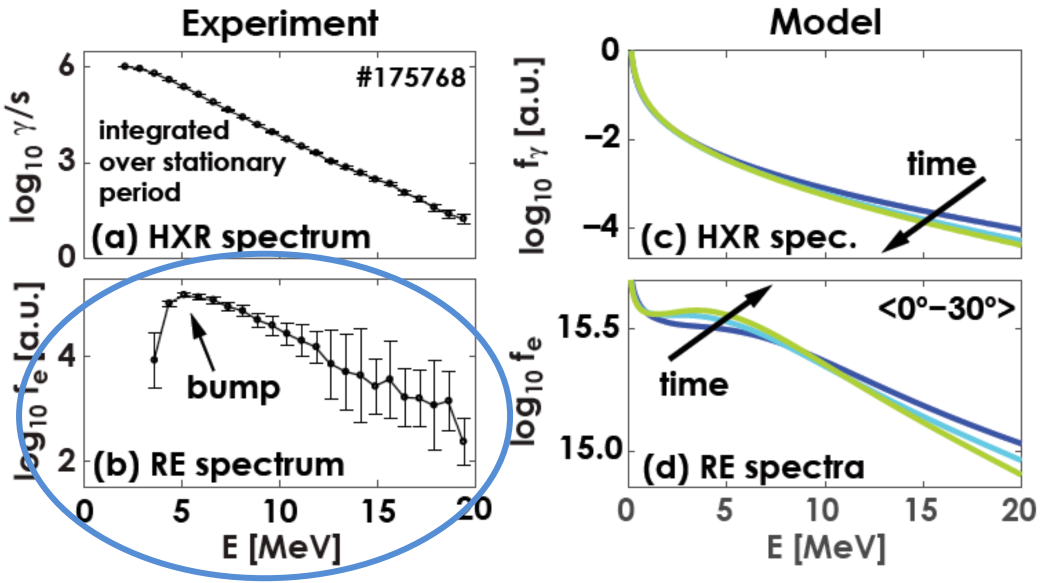


Clear qualitative difference – smeared lines
High E/small λ Ne-like line...
Exp. diagnostic options?

Isolated 4.1485 - 4.8737 nm of $2s^22p^53d/2s^22p^53s \rightarrow 2s^22p^6$ transition of Ne-like Ar (Ar^{+8})

So we have a model – what about a more realistic scenario?

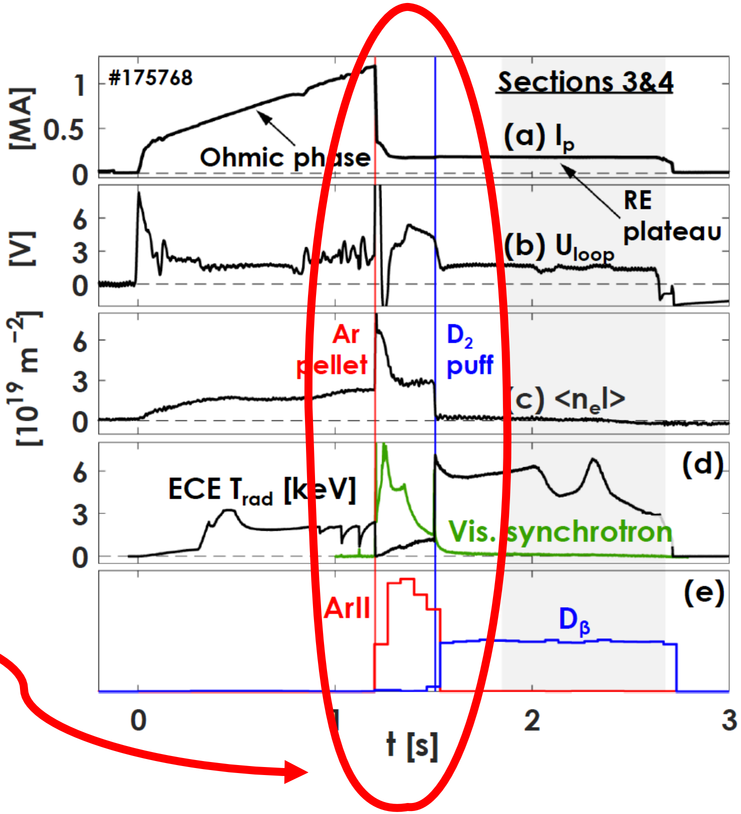
- Experimental point of reference from DIII-D measurements in Lvovskiy *et al.* NF 60 056008 (2020)
- Presents a nice reconstructed f(E) from HXR spectra
- Peak around 5-6 MeV, roll off to approx. 20 MeV



Reproduced from page 4 of Lvovskiy *et al.* NF 60 056008 (2020)

DIII-D-inspired example

- Experimental point of reference [Lvovskiy *et al.* NF 60 056008 (2020)]
- Reconstructed f(E) from HXR spectra
- Simulate conditions prior to D_2 puff – this window of time
- n_D=1.25x10^{19} m^{-3}
- n_{Ar}=2.5x10^{19} m^{-3}
- n_{RE} to produce 180 kA RE current, approx. 10^{16} m^{-3}



Reproduced from page 3 of Lvovskiy *et al.* NF 60 056008 (2020)

Analytic trial functions for DIII-D-inspired f(E)

- Experimental point of reference [Lvovskiy *et al.* NF 60 056008 (2020)]
- Fit f(E) from reconstructed data
- Normalize and align to measured peak
- f_M with T_e=10 MeV*
- f_{MJ} with T_e= 3 MeV
- LSQ fit f_G with μ_E = 5.9 MeV, FWHM = 3.8 MeV*
- LSQ fit f_{BMJ} with p_b=11.3mc, T_e=0.03 MeV
- f_{BMJ} with p_b=10mc T_e=0.07MeV*

$$f_M(E) = \frac{2\sqrt{E}}{\sqrt{\pi}T_e^{1.5}} \exp(-E/T_e)$$

$$f_{MJ}(\gamma) = \frac{\gamma^2\beta}{\theta K_2(1/\theta)} \exp(-\gamma/\theta)$$

$$\theta = T_e/m_e c^2$$

$$f_G(E) = \frac{1}{\sqrt{2\pi}\sigma_E} \exp\left(-\frac{(E-\mu_E)^2}{2\sigma_E^2}\right)$$

$$\sigma_E = \frac{E_{FWHM}}{2\sqrt{2\log 2}}$$

$$f_{BMJ}(p, p_\parallel) = \frac{1}{4\pi\theta\gamma_b K_2(1/\theta)} \exp(-(\gamma_b\gamma(p) - p_b p_\parallel)/\theta)$$

Integrate over pitch

$$f_{BMJ}(p) = \frac{1}{\gamma_b p_b p K_2(1/\theta)} \exp(-\gamma_b\gamma(p)/\theta) \sinh(p_b p/\theta)$$

Analytic trial functions for DIII-D-inspired f(E)

- Experimental point of reference [Lvovskiy *et al.* NF 60 056008 (2020)]
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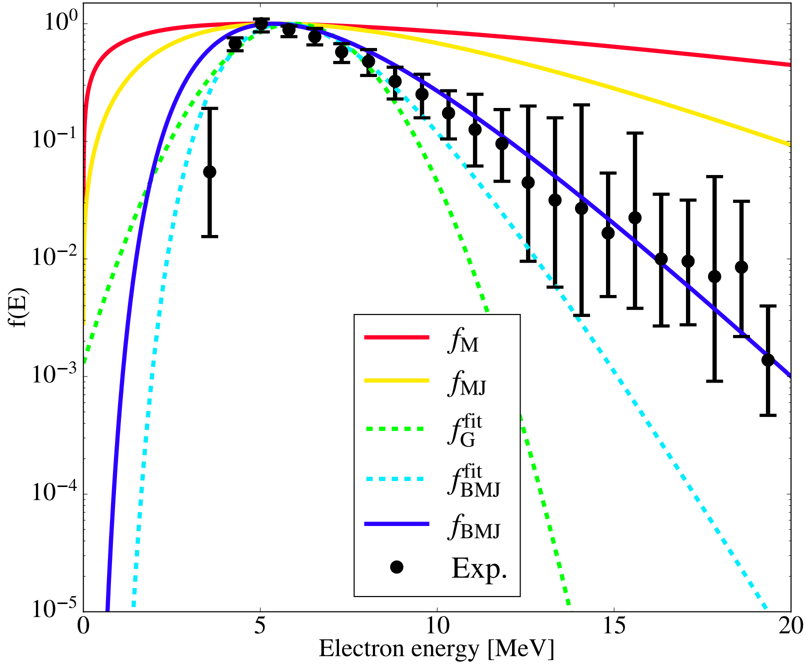
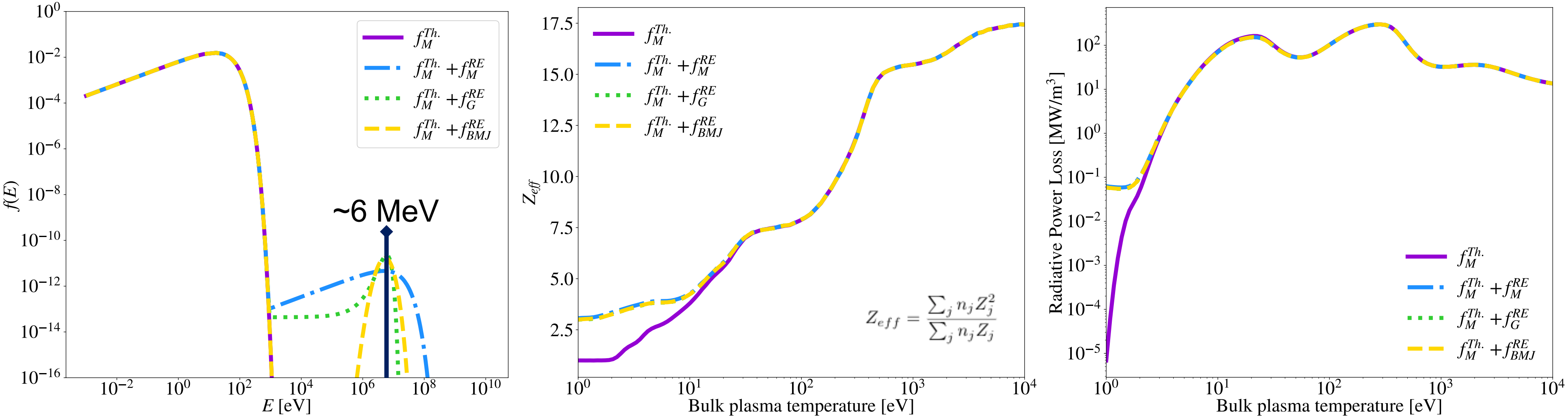


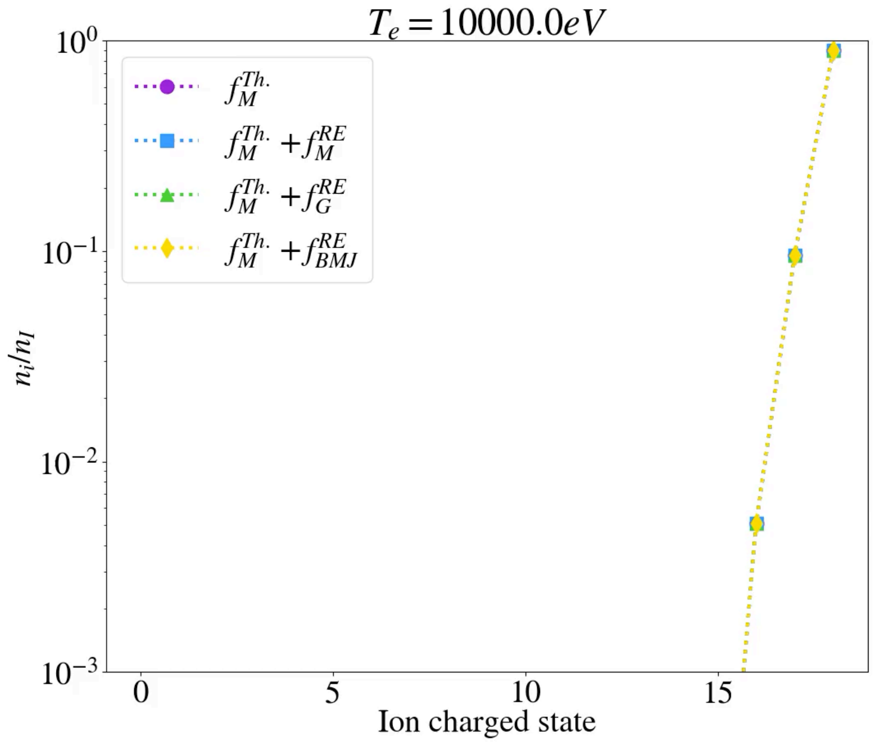
Comparison of different RE f(E) forms

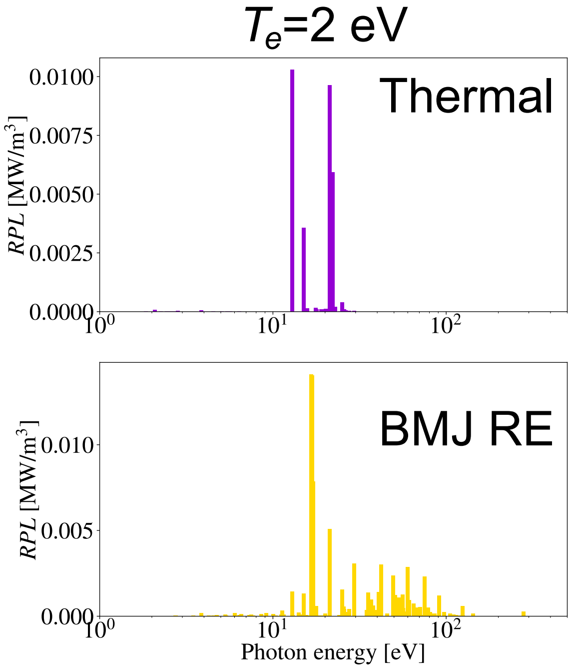
n_D=1.25x10^{19} m^{-3} n_{Ar}=2.5x10^{19} m^{-3} n_{RE} to produce 180 kA RE current



Either Maxwellian*, Gaussian* or boosted Maxwell-Jüttner* seem to perform comparably describing presence of RE tail

Effects of CSD smearing clear





What does a higher n_e and broader set of ion stages mean for runaway electron modeling?

- Translates to different collisional drag/slowing down and pitch-angle scattering/deflection frequencies on RHS of kinetic equation

$$C^{ab} = \nu_D^{ab} \mathcal{L}(f_a) + \frac{1}{p^2}\frac{\partial}{\partial p}\left[p^3\left(\nu_S^{ab} f_a + \frac{1}{2}\nu_\parallel^{ab} p \frac{\partial f_a}{\partial p}\right)\right]$$

  - Consider the formulation of Hesslow *et al. PRL* **118** 25 (2017)

$$\nu_D^{ei} = \nu_{D,\text{cs}}^{ei}\left(1 + \frac{1}{Z_{\text{eff}}}\sum_j \frac{n_j}{n_e}\frac{g_j(p)}{\ln\Lambda}\right)$$

$$\nu_S^{ee} = \nu_{S,\text{cs}}^{ee}\left[1 + \sum_j \frac{n_j N_{e,j}}{n_e \ln\Lambda}\left(\frac{1}{k}\ln\left(1 + h_j^k\right) - \beta^2\right)\right]$$

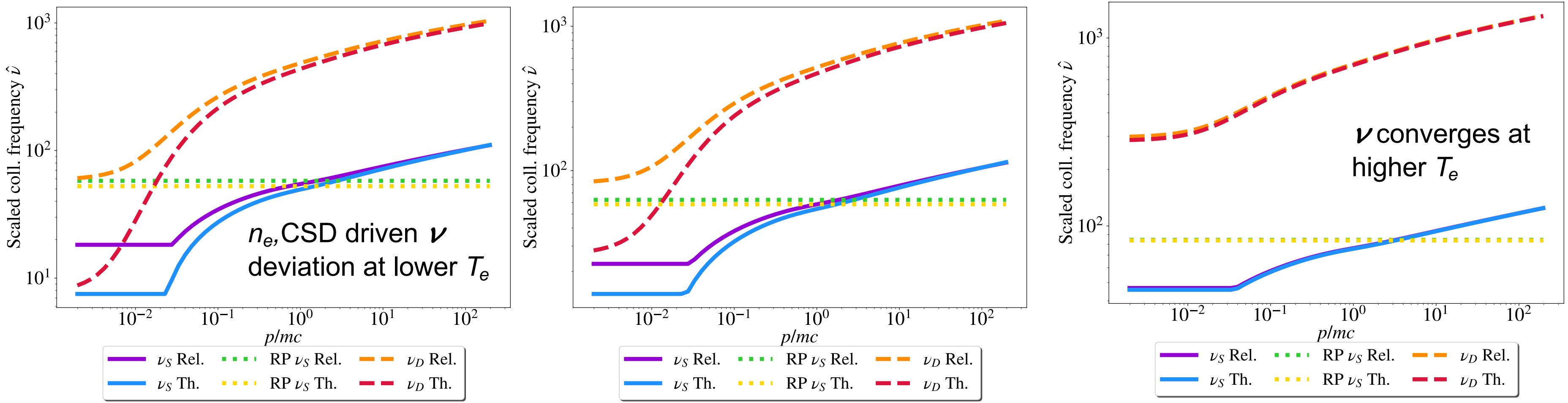
Drag and deflection collision frequencies for RE modeling

- Boosted MJ scenario compared to thermal
- Note: comparing scaled ν to make for clearer comparison

$$\hat{\nu}_S^{ee} = \nu_S^{ee}\frac{p^3}{\gamma^2}$$

$$\hat{\nu}_D^{ei} = \nu_D^{ei}\frac{p^3}{\gamma}$$

T_e=2 eV | T_e=5 eV | T_e=20 eV



RP ν_S Rel.
RP ν_S Th.

$$\nu_{S,\mathrm{RP}}^{ee} \approx \nu_{S,\mathrm{cs}}^{ee}\left[1 + \tfrac{1}{2}\textstyle\sum_j n_j N_{e,j}/n_e\right]$$

A shameless plug before I finish

PoP letter earlier this year – analysis with Gaussian RE tail

Physics of Plasmas LETTER scitation.org/journal/php

Impact of a minority relativistic electron tail interacting with a thermal plasma containing high-atomic-number impurities

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ABSTRACT

A minority relativistic electron component can arise in both laboratory and naturally occurring plasmas. In the presence of high-atomic-number ion species, the ion charge state distribution at a low bulk electron temperature can be dominated by relativistic electrons, even though their density is orders of magnitude lower. This is due to the relativistic enhancement of the collisional excitation and ionization cross sections. The resulting charge state effect can dramatically impact the radiative power loss rate and the related Bethe stopping power of relativistic electrons in a dilute plasma.

\+

Upcoming more detailed paper being prepared for 2020 DPP Special Collection

The takeaway

- Formation of relativistic RE tail is a well known problem for disruptions on ITER
- Atomic physics tells us corrections are needed to normal scattering data and thus CR models used to describe our discharges.
- With minority RE densities driving post-disruption current, influences due to this RE driven physics emerge
- Seems to corroborate apparent observations of low charge states of impurity ions during RE plateau
- **Moving forward:** How can this modeling help guide diagnosing and understanding post-disruption discharges with RE present?

Other avenues in this project

- Improving atomic physics: charge exchange, bencharking ICS
- Time-dependent thermal plasma T_e cooling dynamics
  - Highlighting the importance of excited states and applicability of coronal-like assumptions
- Implementing in-situ for dynamic EEDF in kinetic codes
- Neural network surrogates for rapid evaluation to couple with plasma transport codes (Paper accepted for Machine Learning and the Physical Sciences Workshop at the 34th NeurIPS Conference.)

Thanks for your attention

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- DoE through OFES and the Tokamak Disruption Studies SciDAC
- LDRD program of LANL under project 20200356ER

Questions?