Clog Doc: A_asymtotic_notes1.0.tex

A-Coefficient Study # 1

Robert Singleton

Research Notes
Project:
Clog Doc
Path of TeX Source:
Clog/doc/dedx/A_asymtotic_notes1.0.tex
Last Modified By:
Robert Singleton
3/5/2020
Date Started:
3/5/2020
Date:
v1.0 Thursday 5th March, 2020 07:20

A-Coefficient Study # 1

Robert L Singleton Jr
School of Mathematics
University of Leeds
LS2 9JT

(Dated: 3/5/2020)

Abstract

This is a study of the asymptotic behavior of the $\mathcal{A}$-coefficients from `Clog/acoeff.f90`. Each figure is constructed by a Fortran driver `grXXX.f90` and a corresponding plotting routine `grXXX.sm`. The plasma under consideration is equimolar DT with electron number density n_e, electron temperature T_e, and ion temperature T_I. The code used to generate the data has now been fully checked.

Contents

I. A-COEFFICIENTS AS A FUNCTION OF ENERGY

The A-coefficients take the form

$$\mathcal{A}_b \;=\; \mathcal{A}_b^{\rm C} + \mathcal{A}_b^{\Delta Q} \quad \text{where} \quad \mathcal{A}_b^{\rm C} = \mathcal{A}_{b,{\rm S}}^{\rm C} + \mathcal{A}_{b,{\rm R}}^{<} \;, \tag{1.1}$$

with

$$\mathcal{A}_{b,{\rm S}}^{\rm C} \;=\; \frac{e_p^2\,\kappa_b^2}{4\pi}\left(\frac{\beta_b m_b}{2\pi}\right)^{1/2} v_p \int_0^1 du\, u^{1/2}\, \exp\left\{-\frac{1}{2}\,\beta_b m_b v_p^2\, u\right\} \left[-\ln\left(\beta_b \frac{e_p e_b}{4\pi}\, K\, \frac{m_b}{m_{pb}}\, \frac{u}{1-u}\right) - 2\gamma + 2\right] \tag{1.2}$$

$$\mathcal{A}_{b,{\rm R}}^{<} \;=\; \frac{e_p^2}{4\pi}\,\frac{i}{2\pi}\int_{-1}^{1} d\cos\theta\, \cos\theta\, \frac{\rho_b(v_p\cos\theta)}{\rho_{\rm total}(v_p\cos\theta)}\, F(v_p\cos\theta)\ln\left\{\frac{F(v_p\cos\theta)}{K^2}\right\} \;, \tag{1.3}$$

$$\mathcal{A}_b^{\Delta Q} \;=\; -\frac{e_p^2\,\kappa_b^2}{4\pi}\left(\frac{\beta_b m_b}{2\pi}\right)^{1/2} \frac{1}{2}\int_0^\infty dv_{pb}\left\{2\,{\rm Re}\,\psi\,(1+i\eta_{pb}) - \ln\eta_{pb}^2\right\} \frac{1}{\beta_b m_b v_p v_{pb}}\left[\exp\left\{-\frac{1}{2}\,\beta_b m_b\,(v_p - v_{pb})^2\right\}\left(1 - \frac{1}{\beta_b m_b v_p v_{pb}}\right) + \exp\left\{-\frac{1}{2}\beta_b m_b\,(v_p + v_{pb})^2\right\}\left(1 + \frac{1}{\beta_b m_b v_p v_{pb}}\right)\right] , \tag{1.4}$$

and $\eta_{ab} = e_a e_b/4\pi\hbar v_{ab}$. Figures 1–3 show the $\mathcal{A}$-coefficients for (i) $T_e = T_{\rm I} = 10\,{\rm keV}$, (ii) $T_e = 10\,{\rm keV}$ and $T_{\rm I} = 100\,{\rm keV}$, and (iii) $T_e = 100\,{\rm keV}$ and $T_{\rm I} = 10\,{\rm keV}$ respectively, all with an electron number density $n_e = 10^{25}\,{\rm cm}^{-3}$.

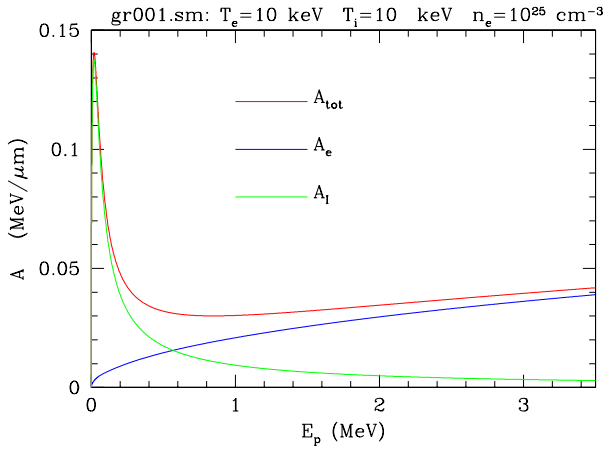

FIG. 1: Electron and ion components: $n_e = 10^{25}\,{\rm cm}^{-3}$, $T_e = 10\,{\rm keV}$, $T_{\rm I} = 10\,{\rm keV}$. [gr001.f90, gr001.sm, gr001.dat, gr001.eps]

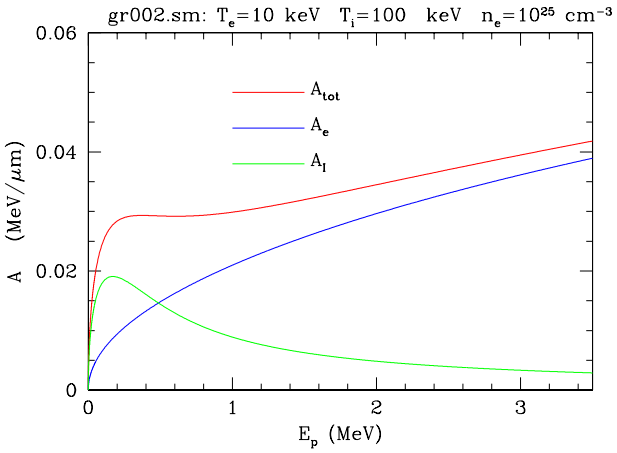

FIG. 2: Electron and ion components: $n_e = 10^{25}\,\mathrm{cm}^{-3}$, $T_e = 10\,\mathrm{keV}$, $T_\mathrm{I} = 100\,\mathrm{keV}$. [gr002.f90, gr002.sm, gr002.dat, gr002.eps]

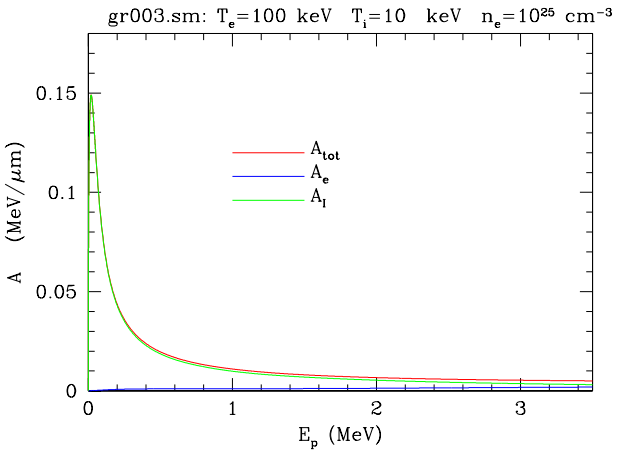

FIG. 3: Electron and ion components: $n_e = 10^{25}\,\mathrm{cm}^{-3}$, $T_e = 100\,\mathrm{keV}$, $T_\mathrm{I} = 10\,\mathrm{keV}$. [gr003.f90, gr003.sm, gr003.dat, gr003.eps]

II. SMALL ENERGY ASYMPTOTIC BEHAVIOR

In the small energy limit, the $\mathcal{A}$-coefficients become:

$$v_p \to 0 \; : \mathcal{A}_b(v_p) = \underbrace{\frac{e_p^2\,\kappa_b^2}{4\pi}}_{c_1} \; \underbrace{\left(\frac{\beta_b m_b}{2\pi}\right)^{1/2} v_p}_{c_2} \cdot \left\{ A_b^{\rm C} + A_b^{\Delta Q} \right\} , \tag{2.1}$$

with

$$A_b^{\rm C} \;=\; \frac{2}{3}\left[\ln\left(\frac{16\pi}{e_p e_b\,\beta_b \kappa_{\rm D}}\,\frac{m_{pb}}{m_b}\right) - \frac{1}{2} - 2\gamma\right] \tag{2.2}$$

$$A_b^{\Delta Q} \;=\; -\bar{\eta}_{pb}^2 \int_0^\infty du\, u\, \exp\left\{-\frac{3}{2}\bar{\eta}_{pb}^2\, u^2\right\}\left[2\,{\rm Re}\,\psi\left(1+\frac{i}{u}\right) + \ln u^2\right] , \tag{2.3}$$

and $\bar{\eta}_{pb} = e_p e_b/4\pi\hbar\bar{v}_b$ (note: $\bar{v}_b^2 = 3T_b/m_b$). The small energy quantum contribution takes separate forms for electrons and ions:

$$\bar{\eta}_{pe}^2 \ll 1 \; : \quad A_e^{\Delta Q} \simeq -\bar{\eta}_{pe}^2 \int_0^\infty du\, u\, \exp\left\{-\frac{3}{2}\bar{\eta}_{pe}^2\, u^2\right\}\left[-2\,\gamma + \ln u^2\right] = \frac{1}{3}\,\ln\left(\frac{3}{2}\,\bar{\eta}_{pe}^2\right) + \gamma\,. \tag{2.4}$$

$$\bar{\eta}_{pi}^2 \gg 1 \; : \quad A_i^{\Delta Q} \simeq -\frac{\bar{\eta}_{pi}^2}{6} \int_0^\infty du\, u^3\, \exp\left\{-\frac{3}{2}\bar{\eta}_{pi}^2\, u^2\right\} = -\frac{1}{27}\,\bar{\eta}_{pi}^{-2}\,. \tag{2.5}$$

The next figure illustrates the relative size of the classical contribution $\mathcal{A}^{\rm C}$ and the total coefficient $\mathcal{A} = \mathcal{A}^{\rm C} + \mathcal{A}^{\rm QM}$. for the density $n_e = 10^{25}\,{\rm cm}^{-3}$. This gives us an idea of the size of the quantum contribution.

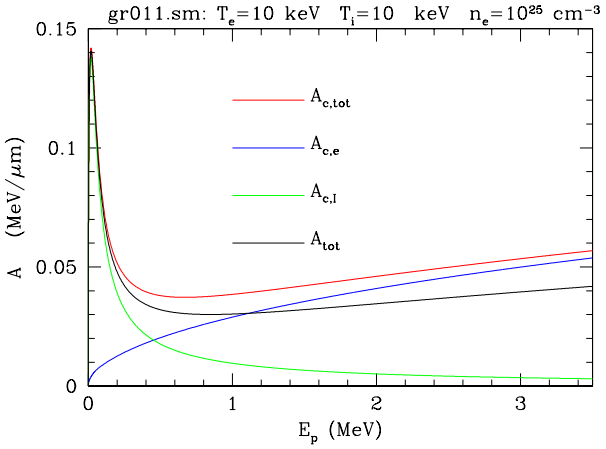

FIG. 4: The classical contributions to the A-coefficient, with the total (classical + quantum) in black. [gr001.f90, gr011.sm, gr001.dat, gr011.eps]

A. Ions: Classical and Quantum

For each of the three cases illustrated in Figs. 1–3, we will now look at the ion contributions for the classical and quantum cases.

1. *Temperatures* $T_e = 10\,\mathrm{keV}$ *and* $T_\mathrm{I} = 10\,\mathrm{keV}$

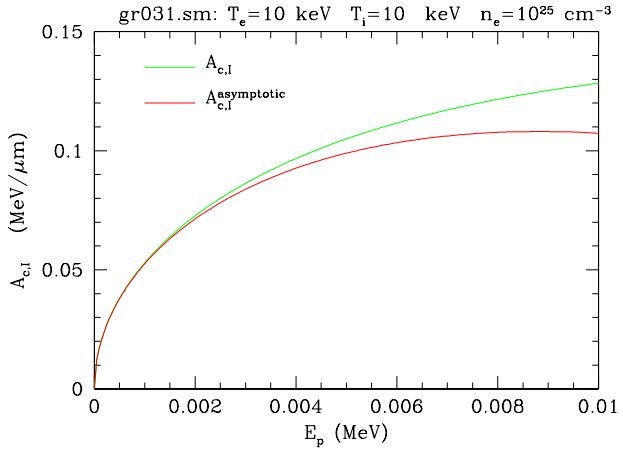

FIG. 5: Asymptotic classical ion contribution at low energies. [gr001.f90, gr031.sm, gr001.dat, gr001.smallE.dat, gr031.eps]

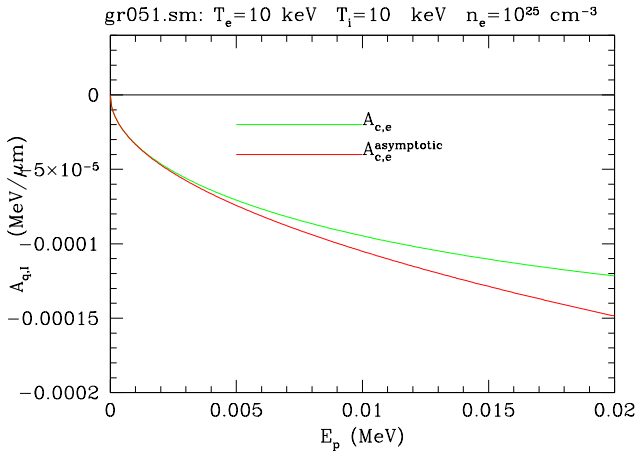

FIG. 6: Asymptotic quantum ion contribution at low energies. [gr001.f90, gr051.sm, gr001.dat, gr001.smallE.dat, gr051.eps]

2. Temperatures $T_e = 10\,\mathrm{keV}$ *and* $T_\mathrm{I} = 100\,\mathrm{keV}$

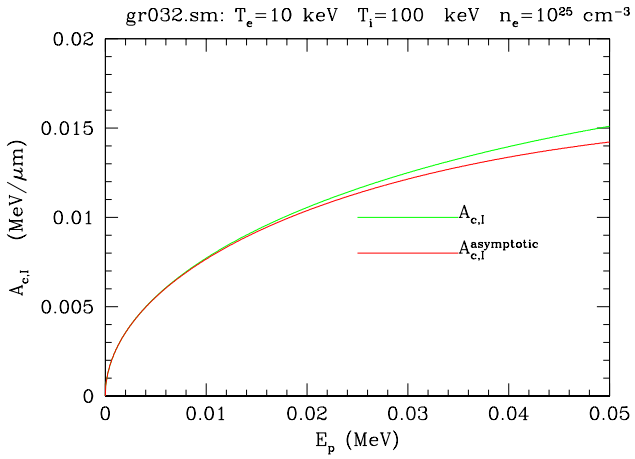

FIG. 7: Asymptotic classical ion contribution at low energies. [gr002.f90, gr032.sm, gr002.dat, gr002.smallE.dat, gr032.eps]

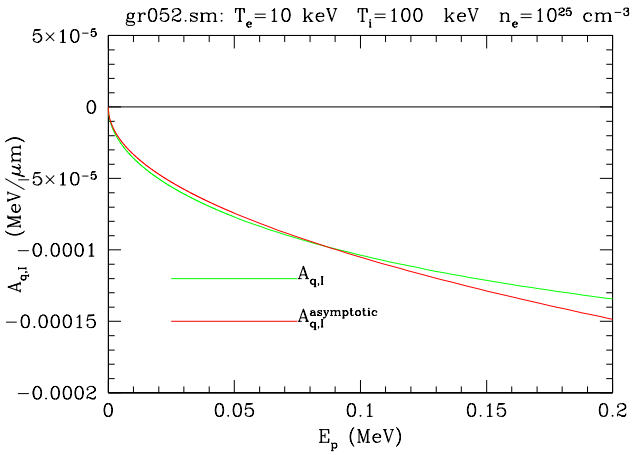

FIG. 8: Asymptotic quantum ion contribution at low energies. [gr002.f90, gr052.sm, gr002.dat, gr002.smallE.dat, gr052.eps]

3. Temperatures $T_e = 100\,\mathrm{keV}$ and $T_\mathrm{I} = 10\,\mathrm{keV}$

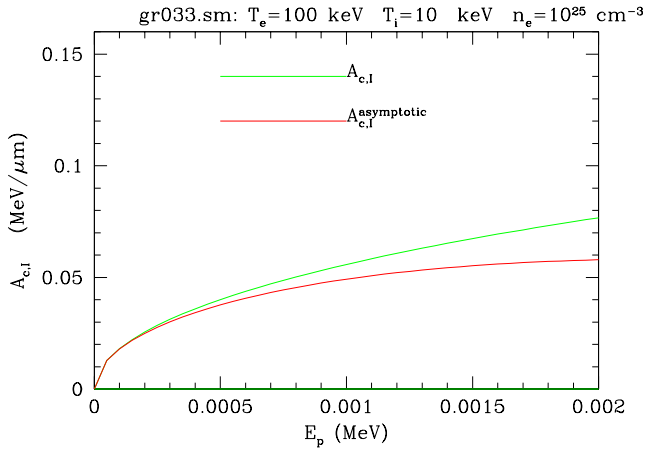

FIG. 9: Asymptotic classical ion contribution at low energies. [gr003.f90, gr033.sm, gr003.dat, gr003.smallE.dat, gr033.eps]

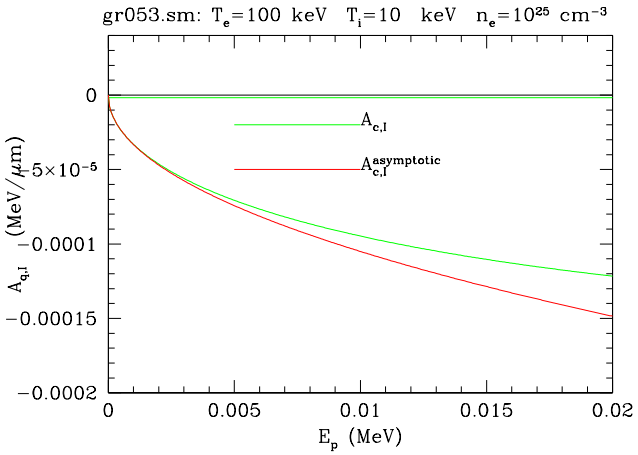

FIG. 10: Asymptotic quantum ion contribution at low energies. [gr003.f90, gr053.sm, gr003.dat, gr003.smallE.dat, gr053.eps]

B. Electrons: Classical and Quantum

For each of the three cases illustrated in Figs. 1–3, we will now look at the electron contributions for the classical and quantum cases.

1. *Temperatures* $T_e = 10\,\mathrm{keV}$ *and* $T_\mathrm{I} = 10\,\mathrm{keV}$

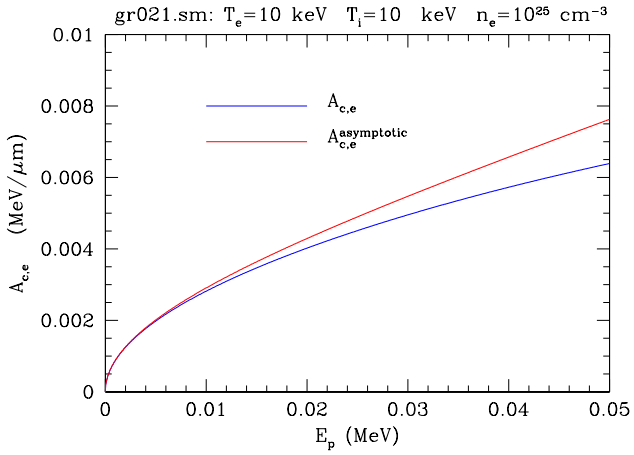

FIG. 11: Asymptotic classical electron contribution at low energies. [gr001.f90, gr021.sm, gr001.dat, gr001.smallE.dat, gr021.eps]

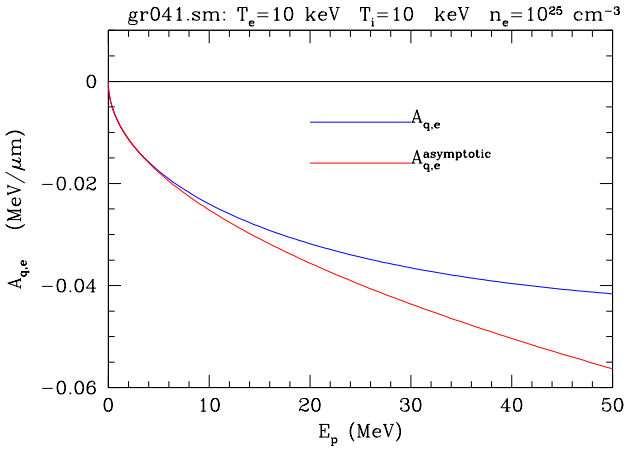

FIG. 12: Asymptotic quantum electron contribution at low energies. [gr001.f90, gr041.sm, gr001.dat, gr001.smallE.dat, gr041.eps]

2. Temperatures $T_e = 10\,\mathrm{keV}$ and $T_\mathrm{I} = 100\,\mathrm{keV}$

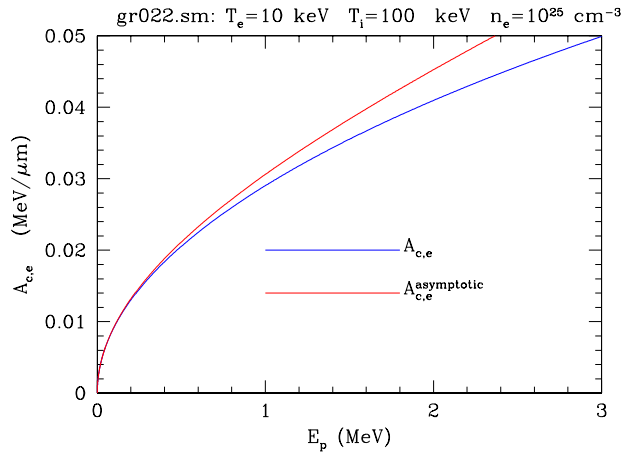

FIG. 13: Asymptotic classical electron contribution at low energies. [gr002.f90, gr022.sm, gr002.dat, gr002.smallE.dat, gr022.eps]

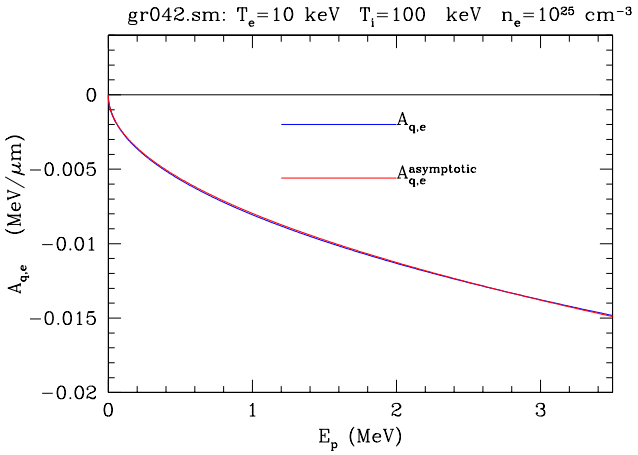

FIG. 14: Asymptotic quantum electron contribution at low energies. [gr002.f90, gr042.sm, gr002.dat, gr002.smallE.dat, gr042.eps]

3. Temperatures $T_e = 100\,\mathrm{keV}$ and $T_\mathrm{I} = 10\,\mathrm{keV}$

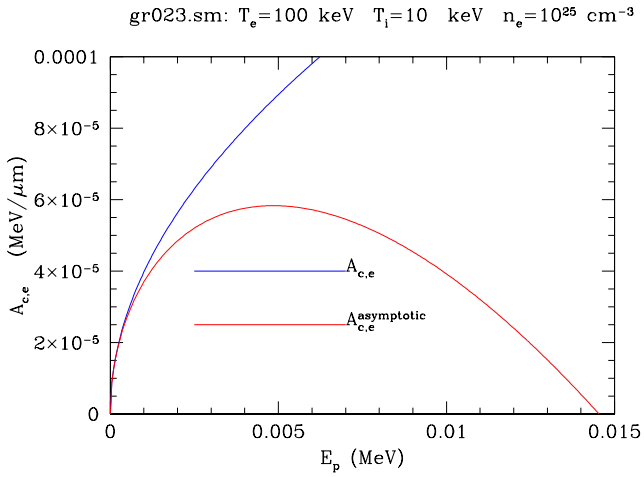

FIG. 15: Asymptotic classical electron contribution at low energies. [gr003.f90, gr023.sm, gr003.dat, gr003.smallE.dat, gr023.eps]

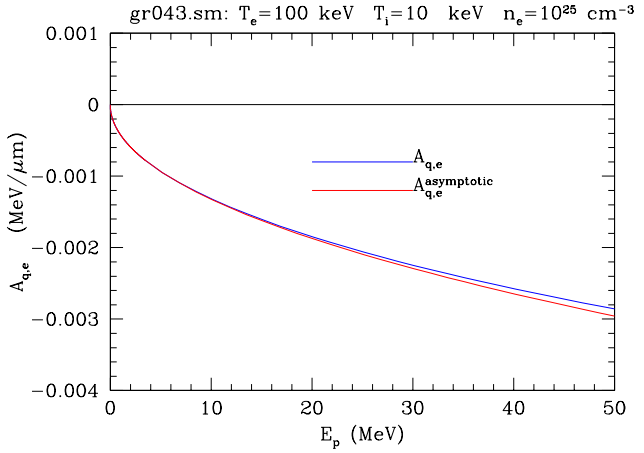

FIG. 16: Asymptotic quantum electron contribution at low energies. [gr003.f90, gr043.sm, gr003.dat, gr003.smallE.dat, gr043.eps]

C. Total Electron and Ion Contributions

1. Temperatures $T_e = 10\,\mathrm{keV}$ and $T_\mathrm{I} = 10\,\mathrm{keV}$

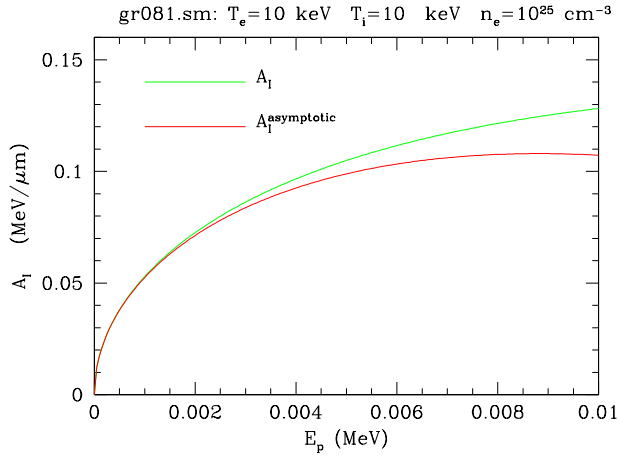

FIG. 17: Total asymptotic ion contribution at low energies. [gr001.f90, gr081.sm, gr001.dat, gr001.smallE.dat, gr081.eps]

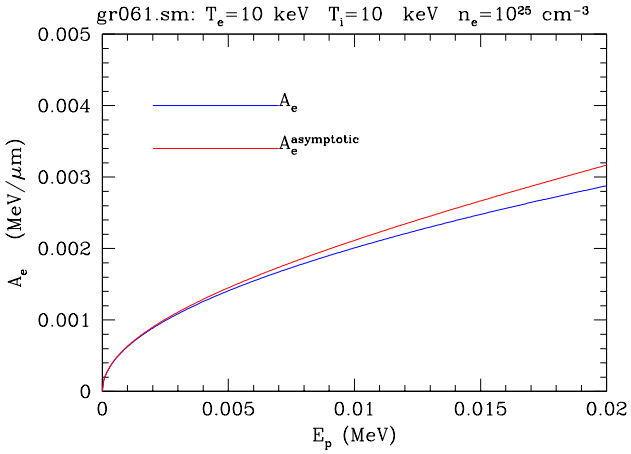

FIG. 18: Total asymptotic electron contribution at low energies. [gr001.f90, gr061.sm, gr001.dat, gr001.smallE.dat, gr061.eps]

2. Temperatures $T_e = 10\,\mathrm{keV}$ *and* $T_\mathrm{I} = 100\,\mathrm{keV}$

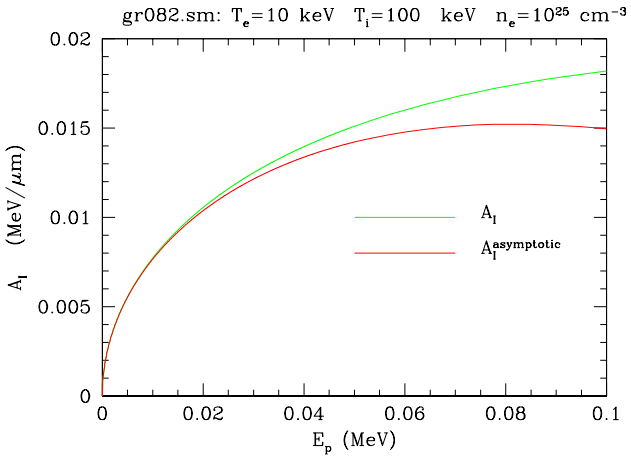

FIG. 19: Total asymptotic ion contribution at low energies. [gr002.f90, gr082.sm, gr002.dat, gr002.smallE.dat, gr082.eps]

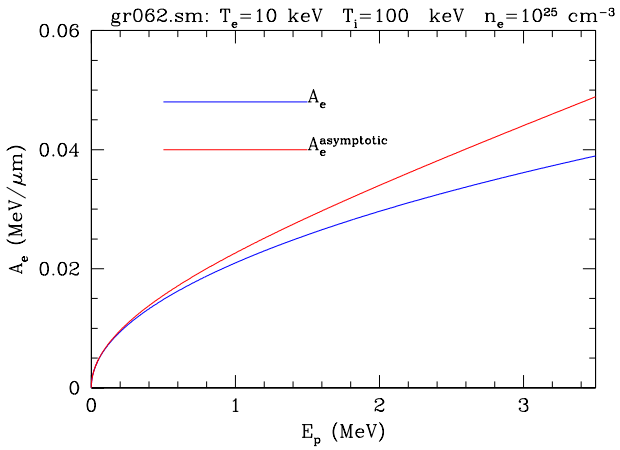

FIG. 20: Total asymptotic electron contribution at low energies. [gr002.f90, gr062.sm, gr002.dat, gr002.smallE.dat, gr062.eps]

3. Temperatures $T_e = 100\,\mathrm{keV}$ and $T_\mathrm{I} = 10\,\mathrm{keV}$

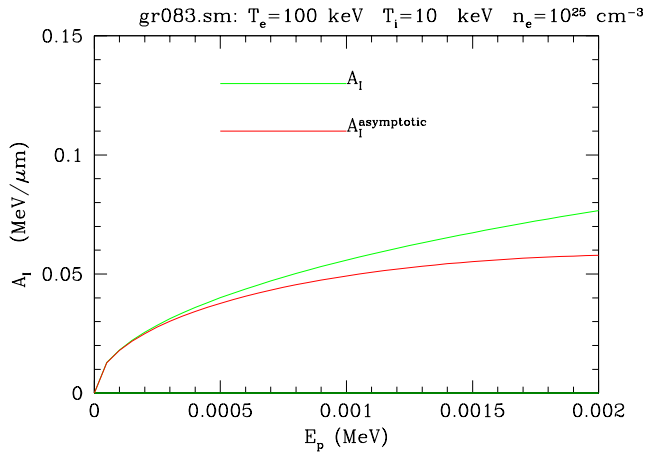

FIG. 21: Total asymptotic ion contribution at low energies. [gr003.f90, gr083.sm, gr003.dat, gr003.smallE.dat, gr083.eps]

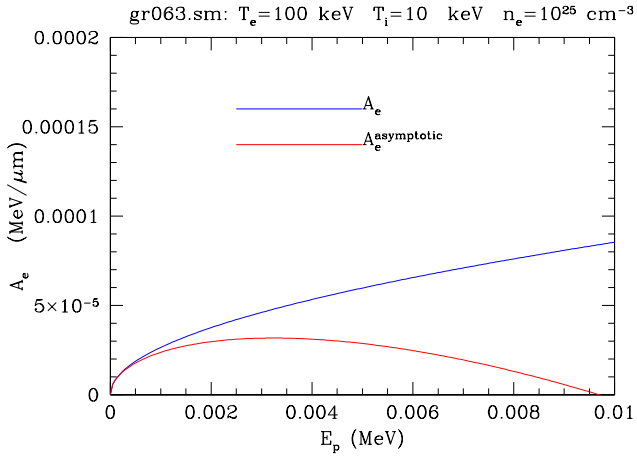

FIG. 22: Total asymptotic electron contribution at low energies. [gr003.f90, gr063.sm, gr003.dat, gr003.smallE.dat, gr063.eps]

III. HIGH ENERGY ASYMPTOTIC BEHAVIOR

A. Ions: Classical and Quantum

We will look at ion contributions before looking at the electrons (this is because there are two high energy electron regimes). For high energy $E \gg T$, the ion contribution to the $\mathcal{A}$-coefficient becomes

$$E_p \gg T : \mathcal{A}_{\rm I}^{\rm C} = \frac{e_p^2}{4\pi}\frac{1}{v_p^2}\sum\nolimits_i \omega_i^2 \left[-\ln\left\{ \frac{e_p e_i \kappa_e}{16\pi}\frac{2}{m_{pi} v_p^2}\right\} - \gamma - \frac{1}{2}\right] \quad \text{[(B36) in text]} \tag{3.1}$$

$$\mathcal{A}_{\rm I}^{\rm QM} = \frac{e_p^2}{4\pi}\frac{1}{v_p^2}\sum\nolimits_i \omega_i^2 \left[-\ln\left\{ \frac{\hbar\kappa_e}{2 m_{pi} v_p}\right\} - \frac{1}{2}\right] . \tag{3.2}$$

To see this, note that the classical singular ion contribution at high energy is given by (B40) [v3.6]:

$$E_p \gg T \quad \eta_{pi} = \frac{e_p e_i}{4\pi\hbar v_p} \gg 1 :$$

$$\mathcal{A}_{i,{\rm S}}^{\rm C} = -\frac{e_p^2}{4\pi}\frac{\omega_i^2}{v_p^2}\left[\ln\left\{ \frac{e_p\, e_i}{16\pi}\frac{2\kappa_e}{m_{pi} v_p^2}\right\} + \gamma\right] \quad \text{[(B40) in text]} \tag{3.3}$$

The regular high energy asymptotic ion term is

$$E_p \gg T\ \ln\left\{ \frac{m_{\rm I} T_e^3}{m_e T_{\rm I}^3}\right\}$$

$$\mathcal{A}_{i,{\rm R}}^{\rm C} = -\frac{e_p^2}{4\pi}\frac{\omega_i^2}{2 v_p^2} \quad \text{[(B34) in text w/o sum]} . \tag{3.4}$$

The asymptotic quantum piece is given by subtracting (B36) for the singular contribution from (B42) [the singular + quantum], to give

$$E_p \gg T : \quad \eta_{pi} = \frac{e_p e_i}{4\pi\hbar\, v_p}$$

$$\mathcal{A}_i^{\rm QM} = \frac{e_p^2}{4\pi}\frac{\omega_i^2}{v_p^2}\left[\ln\eta_{pi} + \gamma\right] \ \text{ note: } \frac{e_p^2}{4\pi}\frac{\omega_i^2}{v_p^2} = \frac{e_p^2\,\kappa_i^2}{4\pi}\frac{\omega_i^2}{\kappa_i^2 v_p^2} = \frac{e_p^2\,\kappa_i^2}{4\pi}\frac{1}{m_i\beta_i v_p^2} . \tag{3.5}$$

The algebra is:

$$\mathcal{A}_i^{\rm QM} = \text{(B42)} - \text{(B36)} \tag{3.6}$$

$$= \frac{e_p^2}{4\pi}\frac{\omega_i^2}{v_p^2}\left[\ln\left\{ \frac{2 m_{pi} v_p}{\hbar\kappa_e}\right\}\right] - \frac{e_p^2}{4\pi}\frac{\omega_i^2}{v_p^2}\left[-\ln\left\{ \frac{e_p e_i \kappa_e}{16\pi}\frac{2}{m_{pi} v_p^2}\right\} - \gamma\right] \tag{3.7}$$

$$= \frac{e_p^2}{4\pi}\frac{\omega_i^2}{v_p^2}\left[\ln\left\{ \frac{2 m_{pi} v_p}{\hbar\kappa_e}\cdot\frac{e_p e_i \kappa_e}{16\pi}\frac{2}{m_{pi} v_p^2}\right\} + \gamma\right] \tag{3.8}$$

$$= \frac{e_p^2}{4\pi}\frac{\omega_i^2}{v_p^2}\left[\ln\left\{ \frac{e_p e_i}{4\pi\,\hbar v_p}\right\} + \gamma\right] . \tag{3.9}$$

1. *Temperatures* $T_e = 10\,\mathrm{keV}$ *and* $T_\mathrm{I} = 10\,\mathrm{keV}$

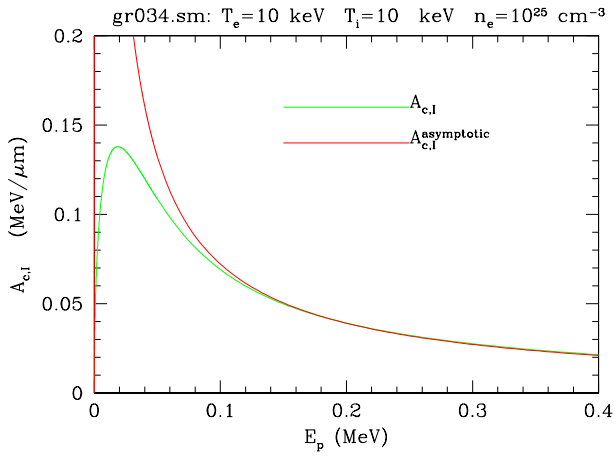

FIG. 23: Asymptotic classical ion contribution at high energies. [gr001.f90, gr034.sm, gr001.dat, gr001.highE.dat, gr034.eps]

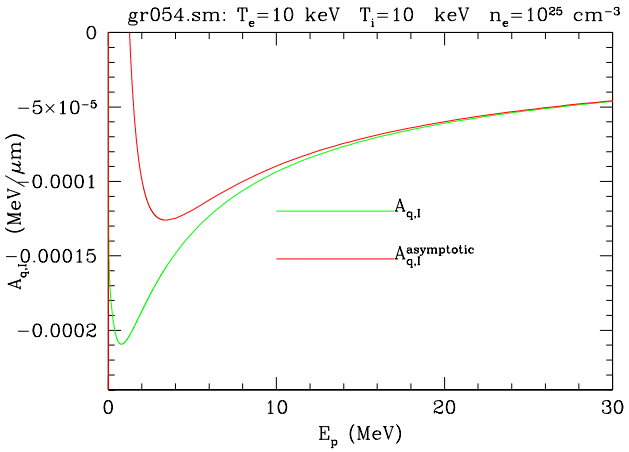

FIG. 24: Asymptotic quantum ion contribution at high energies. [gr001.f90, gr054.sm, gr001.dat, gr001.highE.dat, gr054.eps]

2. *Temperatures* $T_e = 10\,\mathrm{keV}$ *and* $T_\mathrm{I} = 100\,\mathrm{keV}$

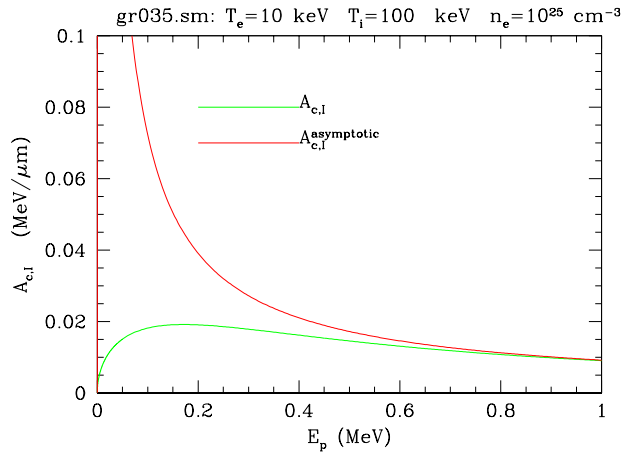

FIG. 25: Asymptotic classical ion contribution at high energies. [gr002.f90, gr035.sm, gr002.dat, gr002.highE.dat, gr035.eps]

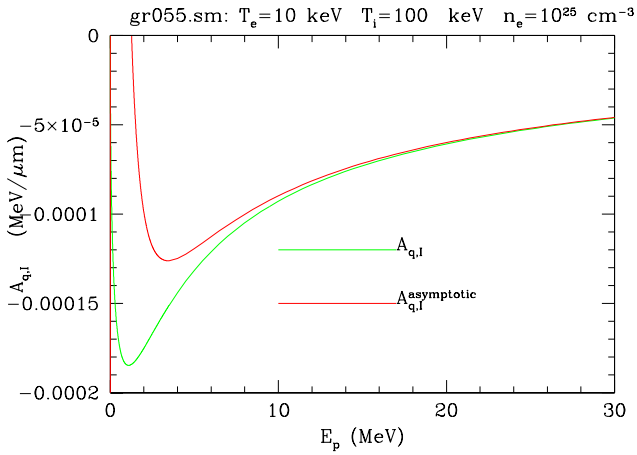

FIG. 26: Asymptotic quantum ion contribution at high energies. [gr002.f90, gr055.sm, gr002.dat, gr002.highE.dat, gr055.eps]

3. Temperatures $T_e = 100\,\mathrm{keV}$ and $T_\mathrm{I} = 10\,\mathrm{keV}$

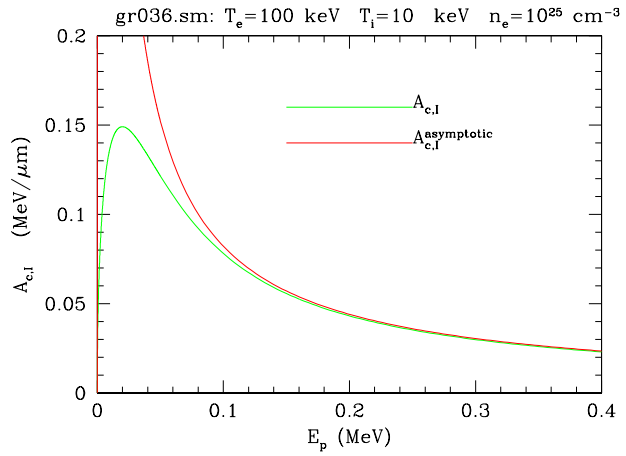

FIG. 27: Asymptotic classical ion contribution at high energies. [gr003.f90, gr036.sm, gr003.dat, gr003.highE.dat, gr036.eps]

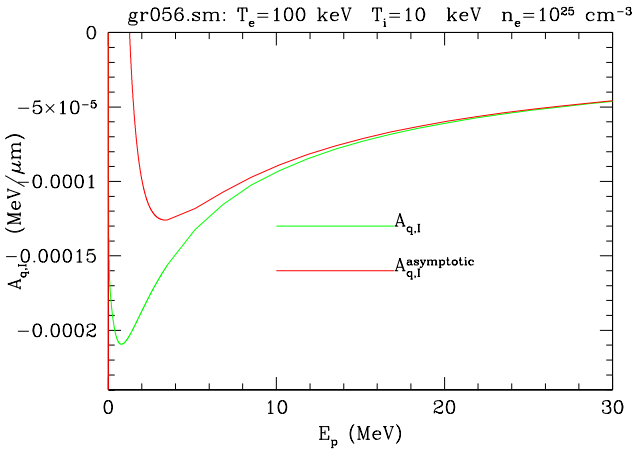

FIG. 28: Asymptotic quantum ion contribution at high energies. [gr003.f90, gr056.sm, gr003.dat, gr003.highE.dat, gr056.eps]

B. Electrons: Classical and Quantum

The high energy electron regime is broken into two widely separated scales, one given by T and the other by $m_{\rm I}T/m_e$. In the high-intermediate energy regime,

$$\frac{m_{\rm I}}{m_e}\,T \gg E_p \gg T: \quad \text{DT plasma at } 10\,\text{keV} \Rightarrow \frac{m_{\rm I\,,\,av}}{m_e}\,T = \frac{2.5\,\text{GeV}}{10\,\text{keV}} = 2.5\,\text{MeV}.$$

$$\mathcal{A}^{<}_{e,\rm R} \;=\; -\frac{e_p^2\,\kappa_e^2}{4\pi}\left(\frac{\beta_e m_e}{2\pi}\right)^{1/2}\frac{v_p}{3}\left[\ln\left\{\frac{\kappa_e^2}{K^2}\right\}+1\right] \quad [\text{ (B51) in text}] \tag{3.10}$$

$$\mathcal{A}^{\rm C}_{e,\rm S}+\mathcal{A}^{\rm QM}_{e} \;=\; \frac{e_p^2\,\kappa_e^2}{4\pi}\left(\frac{\beta_e m_e}{2\pi}\right)^{1/2}\frac{v_p}{3}\left[\ln\left\{\frac{8T_e m_{pe}^2}{m_e\hbar^2K^2}\right\}-\gamma\right] \quad [\text{ (B55) in text}] \tag{3.11}$$

$$\begin{aligned}\mathcal{A}_e \;&=\; \mathcal{A}^{<}_{e,\rm R}+\mathcal{A}^{\rm C}_{e,\rm S}+\mathcal{A}^{\rm QM}_{e}\\ &=\; \frac{e_p^2\,\kappa_e^2}{4\pi}\left(\frac{\beta_e m_e}{2\pi}\right)^{1/2}\frac{v_p}{3}\left[\ln\left\{\frac{8T_e m_{pe}^2}{m_e\hbar^2\kappa_e^2}\right\}-\gamma-1\right] \quad [\text{ (B56) in text}]\,,\end{aligned} \tag{3.12}$$

and in the extreme high energy regime,

$$E_p \gg \frac{m_{\rm I}}{m_e}\,T:$$

$$\mathcal{A}_e \;=\; \frac{e_p^2}{4\pi}\,\frac{\omega_e^2}{v_p^2}\,\ln\left\{\frac{2m_{pe}v_p^2}{\hbar\omega_e}\right\} \quad [\text{ (B58) in text}]\,. \tag{3.13}$$

We now have the total electron contribution $\mathcal{A}_e$ in the extreme and intermediate high energy regimes; however, I will have to calculate $\mathcal{A}^{\rm QM}_e$ later since the text does not give $\mathcal{A}^{\rm C}_{e,\rm S}$ (as it did for the ions).

I will use the coding notation:

$$a_b \;=\; \frac{1}{2}\,\beta_b m_b v_p^2 = \frac{1}{2}\,\beta_b\,m_b c^2\,\left(v_p^2/c^2\right) \tag{3.14}$$

$$c_2 \;=\; \left(\frac{a_e}{\pi}\right)^{1/2} = \left(\frac{\beta_e m_e}{2\pi}\right)^{1/2} v_p = \left(\frac{\beta_e\,m_e c^2}{2\pi}\right)^{1/2}\frac{v_p}{c} \tag{3.15}$$

$$c_1 \;=\; \frac{e_p^2\,\kappa_e^2}{4\pi} = Z_p^2\cdot\frac{e^2}{8\pi a_0}\cdot 2a_0\cdot\kappa_e^2 = 2Z_p^2\,B_e\,\kappa_e^2 a_0\,. \tag{3.16}$$

For coding purposes, the extreme high energy electron contribution can then be written,

$$\mathcal{A}_e \;=\; c_1\,\frac{\omega_e^2}{\kappa_e^2\,v_p^2}\ln\left\{\frac{2\,(m_{pe}c^2)v_p^2}{(\hbar c)\,c\,\omega_e}\right\} = \frac{c_1}{\beta_e m_e v_p^2}\ln\left\{\frac{2\,(m_{pe}c^2)v_p^2}{(\hbar c)\,c\,\omega_e}\right\} \tag{3.17}$$

$$=\; \frac{c_1}{2a_e}\ln\left\{\frac{2\,(m_{pe}c^2)v_p^2}{(\hbar c)\,c\,\omega_e}\right\} \quad \text{(B58)}\,, \tag{3.18}$$

and the intermediate high energy form is

$$\mathcal{A}_e \;=\; \frac{c_1\,c_2}{3}\left[\ln\left\{\frac{8T_e\,(m_{pe}c^2)^2}{(m_e c^2)(\hbar c)^2\,\kappa_e^2}\right\}-\gamma-1\right] \quad \text{(B56)}\,. \tag{3.19}$$

1. Temperatures $T_e = 10\,\mathrm{keV}$ and $T_\mathrm{I} = 10\,\mathrm{keV}$

FIG. 29: Asymptotic classical electron contribution at high energies. [gr001.f90, gr024.sm, gr001.dat, gr001.highE.dat, gr024.eps]

FIG. 30: Asymptotic quantum electron contribution at high energies. [gr001.f90, gr044.sm, gr001.dat, gr001.highE.dat, gr044.eps]

2. Temperatures $T_e = 10\,\mathrm{keV}$ and $T_\mathrm{I} = 100\,\mathrm{keV}$

FIG. 31: Asymptotic classical electron contribution at high energies. [gr002.f90, gr025.sm, gr002.dat, gr002.highE.dat, gr025.eps]

FIG. 32: Asymptotic quantum electron contribution at high energies. [gr002.f90, gr045.sm, gr002.dat, gr002.highE.dat, gr045.eps]

3. Temperatures $T_e = 100\,\mathrm{keV}$ and $T_\mathrm{I} = 10\,\mathrm{keV}$

FIG. 33: Asymptotic classical electron contribution at high energies. [gr003.f90, gr026.sm, gr003.dat, gr003.highE.dat, gr026.eps]

FIG. 34: Asymptotic quantum electron contribution at high energies. [gr003.f90, gr046.sm, gr003.dat, gr003.highE.dat, gr046.eps]

C. Total Electron and Ion Contributions

1. Temperatures $T_e = 10\,\mathrm{keV}$ and $T_\mathrm{I} = 10\,\mathrm{keV}$

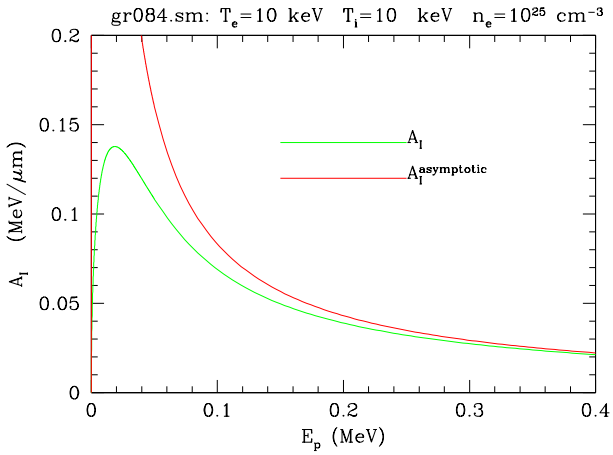

FIG. 35: Total asymptotic ion contribution at high energies. [gr001.f90, gr084.sm, gr001.dat, gr001.highE.dat, gr084.eps]

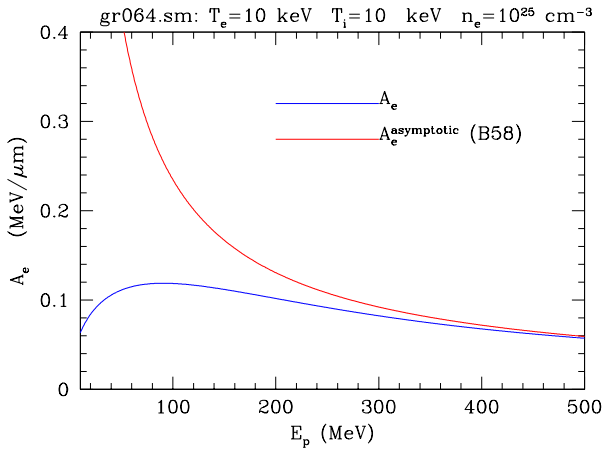

FIG. 36: Total asymptotic electron contribution (B58) at very high energies. [gr001.f90, gr064.sm, gr001.dat, gr001.highEe.dat, gr064.eps]

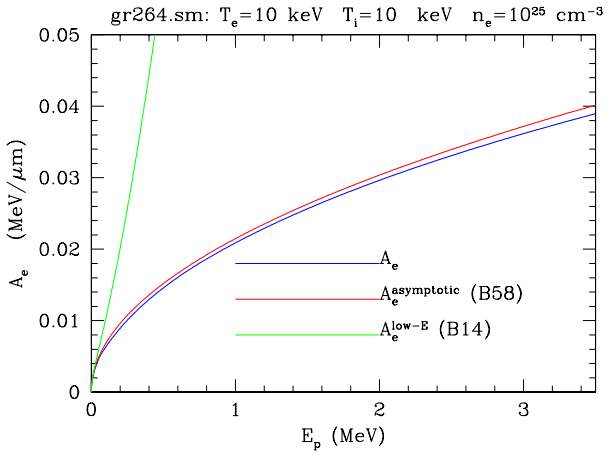

FIG. 37: Total asymptotic electron contribution (B56) at medium high energies. [gr001.f90, gr264.sm, gr001.dat, gr001.highE.dat, gr264.eps]

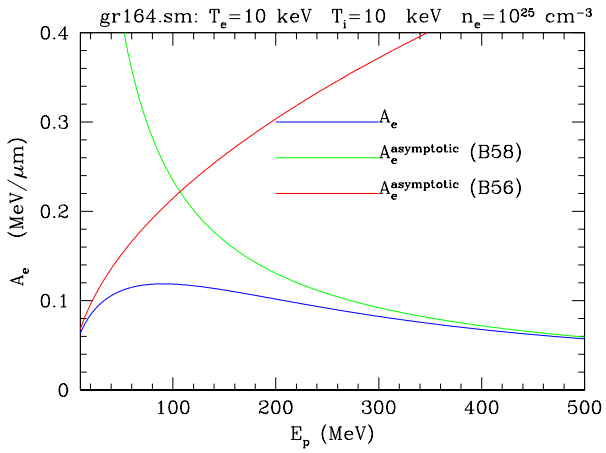

FIG. 38: Total asymptotic electron contribution (B56) and (B58). [gr001.f90, gr164.sm, gr001.dat, gr001.highE.dat, gr001.highEe.dat, gr164.eps]

2. Temperatures $T_e = 10\,\mathrm{keV}$ and $T_\mathrm{I} = 100\,\mathrm{keV}$

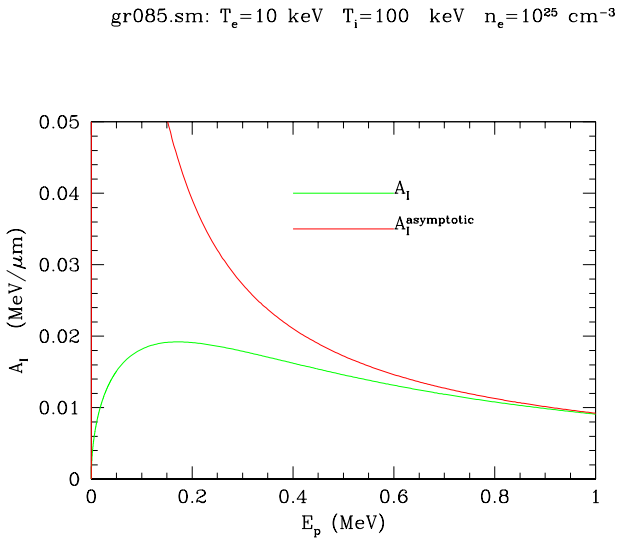

FIG. 39: Total asymptotic ion contribution at high energies. [gr002.f90, gr085.sm, gr002.dat, gr002.highE.dat, gr085.eps]

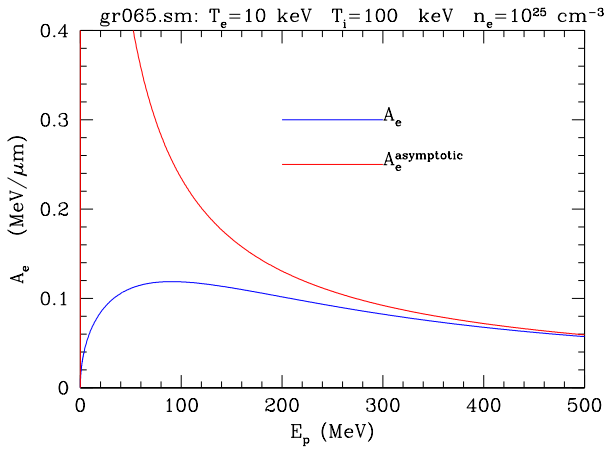

FIG. 40: Total asymptotic electron contribution (B58) at very high energies. [gr002.f90, gr065.sm, gr002.dat, gr002.highE.dat, gr065.eps]

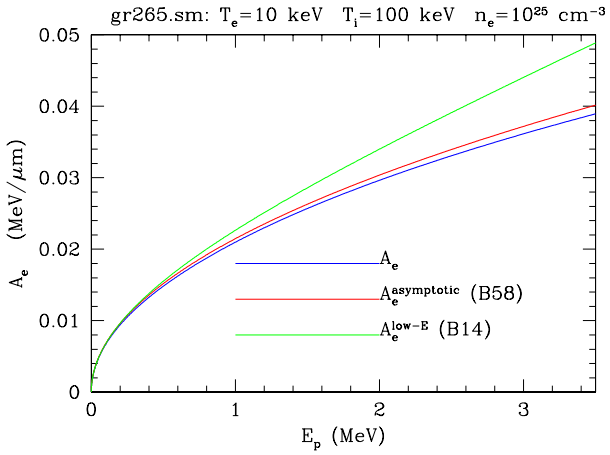

FIG. 41: Total asymptotic electron contribution (B56) at medium high energies. [gr002.f90, gr265.sm, gr002.dat, gr002.highE.dat, gr265.eps]

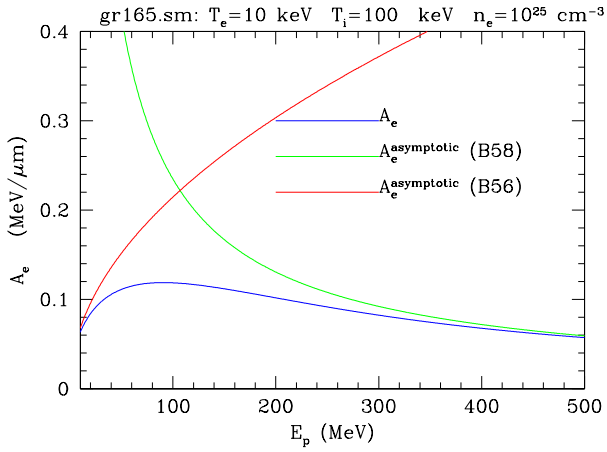

FIG. 42: Total asymptotic electron contribution (B56) and (B58). [gr002.f90, gr165.sm, gr002.dat, gr002.highE.dat, gr002.highEe.dat, gr165.eps]

3. Temperatures $T_e = 100\,\mathrm{keV}$ and $T_\mathrm{I} = 10\,\mathrm{keV}$

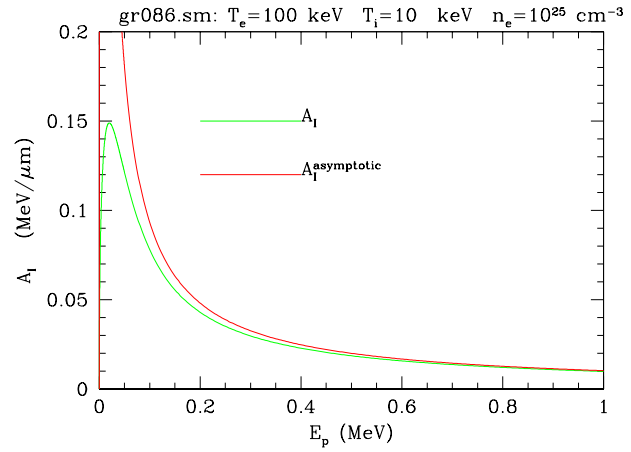

FIG. 43: Total asymptotic ion contribution at high energies. [gr003.f90, gr086.sm, gr003.dat, gr003.highE.dat, gr086.eps]

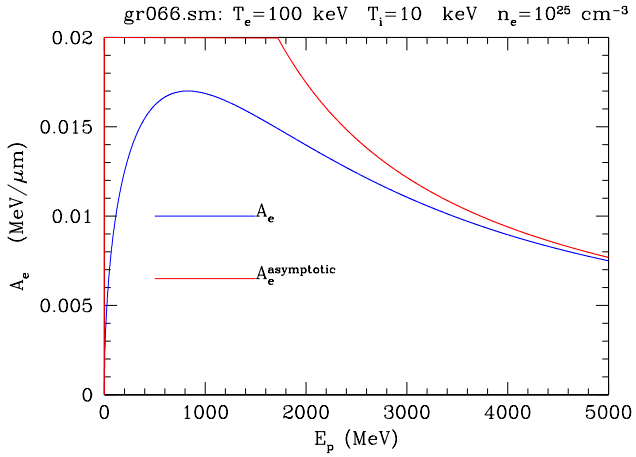

FIG. 44: Total asymptotic electron contribution (B58) at very high energies. [gr003.f90, gr066.sm, gr003.dat, gr003.highEe.dat, gr066.eps]

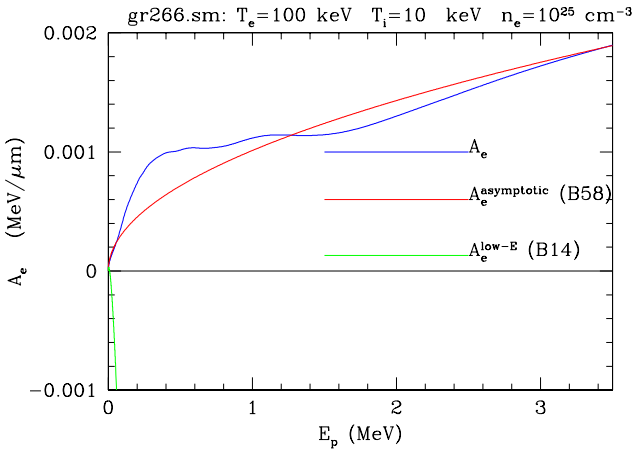

FIG. 45: Total asymptotic electron contribution (B56) at medium high energies. [gr003.f90, gr266.sm, gr003.dat, gr003.highE.dat, gr266.eps]

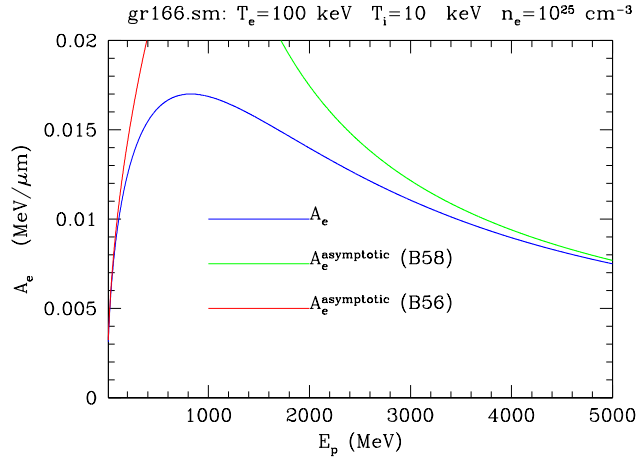

FIG. 46: Total asymptotic electron contribution (B56) at medium high energies. [gr003.f90, gr166.sm, gr003.dat, gr003.highE.dat, gr003.highEe.dat, gr166.eps]

Appendix A: Coding the A-coefficients

1. The Singular Contribution

The singular contribution,

$$\mathcal{A}^{\rm C}_{b,{\rm S}} \;=\; \left[\frac{e_p^2\,\kappa_b^2}{4\pi}\left(\frac{\beta_b m_b}{2\pi}\right)^{1/2} v_p\right]\int_0^1 du\,u^{1/2}e^{-\frac{1}{2}\,\beta_b m_b v_p^2\,u}\left[-\ln\left\{\frac{\beta_b e_b e_p}{4\pi}\,K\,\frac{m_b}{m_{pb}}\,\frac{u}{1-u}\right\}-2\gamma+2\right], \tag{A1}$$

is quite easy to code. The integral can be broke into the pieces

$$\int_0^1 du\,u^{1/2}e^{-\frac{1}{2}\,\beta_b m_b v_p^2\,u}\left[\ln\left\{\frac{u}{1-u}\right\}-\ln\left\{\frac{\beta_b e_b e_p}{4\pi}\,K\,\frac{m_b}{m_{pb}}\right\}-2\gamma+2\right], \tag{A2}$$

which motivates the definition

$$\mathcal{A}^{\rm C}_{b,{\rm S}} \;=\; c_{b,1}\,c_{b,2}\cdot \mathsf{A}_{\rm S}(a_{pb},b_{pb}) \tag{A3}$$

$$\mathsf{A}_{\rm S}(a,b) \;=\; \int_0^1 du\,u^{1/2}e^{-a\,u}\left[-\ln\left\{\frac{u}{1-u}\right\}+b\right] \tag{A4}$$

$$a_{pb} \;=\; \frac{1}{2}\,\beta_b m_b v_p^2 \qquad \text{and} \qquad b_{pb}=-\ln\left\{\frac{\beta_b e_b e_p}{4\pi}\,K\,\frac{m_b}{m_{pb}}\right\}-2\gamma+2 \tag{A5}$$

$$c_{b,1} \;=\; \frac{e_p^2\,\kappa_b^2}{4\pi} \qquad c_{b,2}=\left(\frac{\beta_b m_b}{2\pi}\right)^{1/2} v_p\;. \tag{A6}$$

The term involving b can be integrated exactly, but we will use Gaussian quadrature for both pieces.

acoeff.f90:

```
FUNCTION dab_sing(u, a, b)
  IMPLICIT NONE  ! a=(1/2)*beta*mpc2*vp^2/C^2
  REAL,         INTENT(IN)  :: u ! [dimensionless]
  REAL,         INTENT(IN)  :: a ! [dimensionless]
  REAL,         INTENT(IN)  :: b ! [dimensionless]
  REAL                      :: dab_sing ! [dimensionless]
  dab_sing=SQRT(u)*EXP(-a*u)*(-LOG(u/(1-u)) + b)
END FUNCTION dab_sing
```

The numerical integration is performed by Gaussian quadrature:

acoeff.f90:

```
  SUBROUTINE a_sing(a, b, ac_s)
    REAL,    INTENT(IN)  :: a
    REAL,    INTENT(IN)  :: b
    REAL,    INTENT(OUT) :: ac_s
    REAL                 :: u0, u1, du, u, um
    INTEGER, PARAMETER :: NS=1000           ! integration regions singular: must
    REAL,    PARAMETER :: UPM=0.7745966692E0 ! parameters for Gaussian Quad
    REAL,    PARAMETER :: W13=0.5555555556E0, W2=0.8888888889E0
       ac_s=0
```

```
      u0=0
      u1=1
      du=(u1-u0)/NS
      u=u0-du
      DO iu=1,NS,2 ! Gaussian quadrature
         u=u+2.E0*du
         ac_s=ac_s+W2*dab_sing(u,a,b)
         um=u-du*UPM
         ac_s=ac_s+W13*dab_sing(um,a,b)
         um=u+du*UPM
         ac_s=ac_s+W13*dab_sing(um,a,b)
      ENDDO
      ac_s=ac_s*du
END SUBROUTINE a_sing
```

2. The Regular Contribution

The long-distance regular contribution can be expressed as

$$\mathcal{A}^{<}_{b,\mathrm{R}} \;=\; \frac{e_p^2}{4\pi}\frac{i}{2\pi}\int_{-1}^{1} du\, u\, \frac{\rho_b(v_p u)}{\rho_{\mathrm{total}}(v_p u)}\, F(v_p u) \ln\left\{\frac{F(v_p u)}{K^2}\right\} \tag{A7}$$

$$\;=\; \frac{e_p^2}{4\pi}\frac{i}{2\pi}\int_{0}^{1} du\, u\, \frac{\rho_b(v_p u)}{\rho_{\mathrm{total}}(v_p u)}\, \left[F(v_p u) \ln\left\{\frac{F(v_p u)}{K^2}\right\} - F^*(v_p u) \ln\left\{\frac{F^*(v_p u)}{K^2}\right\}\right] \tag{A8}$$

$$\;=\; -\frac{e_p^2}{4\pi}\frac{1}{2\pi}\int_{0}^{1} du\, u\, \frac{\rho_b(v_p u)}{\rho_{\mathrm{total}}(v_p u)}\, H(v_p u)\ , \tag{A9}$$

where we have defined

$$H(v) \;\equiv\; -i\left[F(v)\ln\left\{\frac{F(v)}{K^2}\right\} - F^*(v)\ln\left\{\frac{F^*(v)}{K^2}\right\}\right] = 2\left[F_{\mathrm{Re}}\arg\{F\} + F_{\mathrm{Im}}\ln\left\{\frac{|F|}{K^2}\right\}\right]\ . \tag{A10}$$

We shall factor out a dimensionfull wavenumber K and define dimensionless quantities $\mathbb{F}(v)$ and $\mathbb{H}(v)$ through

$$F(v) \;=\; K^2\,\mathbb{F}(v) \quad \text{and} \quad H(v) = K^2\,\mathbb{H}(v)\ . \tag{A11}$$

Defining the parameters

$$a_c \;\equiv\; \left(\frac{\beta_c m_c}{2}\right)^{1/2} \tag{A12}$$

$$\bar{\kappa}_c^2 \;\equiv\; \frac{\kappa_c^2}{K^2} \tag{A13}$$

gives the real and imaginary parts of $\mathbb{F}$,

$$\mathbb{F}_{\mathrm{Re}}(\{a_c v\},\{\bar{\kappa}_c\}) \;=\; \sum\nolimits_c \bar{\kappa}_c^2\Big(1 - 2a_c\, v\, \mathrm{daw}\{a_c\, v\}\Big) \tag{A14}$$

$$\mathbb{F}_{\mathrm{Im}}(\{a_c v\},\{\bar{\kappa}_c\}) \;=\; \sqrt{\pi}\sum\nolimits_c \bar{\kappa}_c^2\, a_c v\, e^{-a_c^2 v^2}\ . \tag{A15}$$

The ratio of weighting factors can be written

$$\frac{\kappa_b^2}{K^2}\,\mathbb{R}_b(\{(u\,\beta_c m_c v_p^2/2)^{1/2}\}) \equiv \frac{\rho_b(v_p u)}{\rho_{\rm total}(v_p u)} = \frac{\kappa_b^2\,(\beta_b m_b/2\pi)^{1/2}\;v_p u\,e^{-\frac{1}{2}\,\beta_b m_b v_p^2\,u^2}}{\sum_c \kappa_c^2\,(\beta_c m_c/2\pi)^{1/2}\;v_p u\,e^{-\frac{1}{2}\,\beta_c m_c v_p^2\,u^2}} \tag{A16}$$

$$= \left[\sum\nolimits_c \frac{\kappa_c^2}{\kappa_b^2}\left(\frac{\beta_c m_c}{\beta_b m_b}\right)^{1/2} e^{\frac{1}{2}\,(\beta_b m_b-\beta_c m_c)v_p^2\,u^2}\right]^{-1}, \tag{A17}$$

or

$$\mathbb{R}_b(\{(u\,\beta_c m_c v_p^2/2)^{1/2}\}) = \left[\sum\nolimits_c \frac{\kappa_c^2}{K^2}\left(\frac{\beta_c m_c}{\beta_b m_b}\right)^{1/2} e^{\frac{1}{2}\,(\beta_b m_b-\beta_c m_c)v_p^2\,u^2}\right]^{-1}. \tag{A18}$$

We can now express the regular piece as

$$\mathcal{A}^{\rm C}_{b,{\rm R}} = \underbrace{\left[\frac{e_p^2\,\kappa_b^2}{4\pi}\right]}_{c_{b,1}} \cdot \mathsf{A}_{\rm R}(v_p,\{a_c\},\{\bar\kappa_c\}) \tag{A19}$$

$$\mathsf{A}_{b\,{\rm R}}(v_p,\{a_c\},\{\bar\kappa_c\}) = \int_0^1 du\;\underbrace{\mathbb{R}_b(\{a_c v_p u\})\,\mathbb{H}(\{a_c\,v_p u\},\{\bar\kappa_c\})}_{\rm dab\_reg}\,. \tag{A20}$$

acoeff.f90:

```
      FUNCTION dab_reg(u, vp, ib, nni, k2, kb2, betab, mb)
      USE mathvars
      USE physvars
        IMPLICIT NONE
        REAL,                          INTENT(IN)  :: u       !  [dimensionless]
        REAL,                          INTENT(IN)  :: vp      !  Projectile velocity [c
        INTEGER,                       INTENT(IN)  :: ib      !  Species number
        INTEGER,                       INTENT(IN)  :: nni     !  Number of ion species
        REAL,                          INTENT(IN)  :: k2      !  Wavenumber squared [1/
        REAL,    DIMENSION(1:nni+1),   INTENT(IN)  :: kb2     !  Debye wavenumber squar
        REAL,    DIMENSION(1:nni+1),   INTENT(IN)  :: betab   !  Temperature array [1/k
        REAL,    DIMENSION(1:nni+1),   INTENT(IN)  :: mb      !  Mass array [keV]
        REAL                                       :: dab_reg !  [dimensionless]
        REAL,    DIMENSION(1:nni+1) :: alfb, ab
        REAL                        :: fr, fi, fabs, farg, h
        REAL                        :: kcb, r_ib, bm_ic, bm_ib, a_ic, a_ib, ex, au
        INTEGER                     :: ic
        ab=SQRT(0.5*betab*mb)*vp/CC
        alfb=kb2/k2
        CALL frfi(u,nni,alfb,ab,fr,fi,fabs,farg)
        h=2*(fr*farg + fi*LOG(fabs))
!
! construct spectral weight ratio Rb=rho_b/rho_tot
!
        r_ib=0
        bm_ib=betab(ib)*mb(ib)
        a_ib =ab(ib)*ab(ib)
        DO ic=1,nni+1
           kcb=kb2(ic)/k2
           bm_ic=betab(ic)*mb(ic)
```

```
      a_ic =ab(ic)*ab(ic)
      IF (ic == ib) THEN
         ex=1
      ELSE
         au=(a_ic-a_ib)*u
         ex=EXP(-au)
      ENDIF
      r_ib=r_ib + kcb*SQRT(bm_ic/bm_ib)*ex
    ENDDO
    r_ib=1/r_ib
    dab_reg=-u*r_ib*h/TWOPI
  END FUNCTION dab_reg
```

The numerical integration is performed by Gaussian quadrature:

acoeff.f90:

```
  SUBROUTINE a_reg(ib, nni, vp, k2, kb2, betab, mb, ac_r)
    INTEGER,                       INTENT(IN)  :: ib
    INTEGER,                       INTENT(IN)  :: nni
    REAL,                          INTENT(IN)  :: k2
    REAL,                          INTENT(IN)  :: kb2
    REAL,    DIMENSION(1:nni+1),   INTENT(IN)  :: betab
    REAL,    DIMENSION(1:nni+1),   INTENT(IN)  :: mb
    REAL,                          INTENT(OUT) :: ac_r
    REAL                 :: u0, u1, du, u, um
    INTEGER, PARAMETER :: NR=10            ! integration regions singular: must b
    REAL,    PARAMETER :: UPM=0.7745966692E0 ! parameters for Gaussian Quad
    REAL,    PARAMETER :: W13=0.5555555556E0, W2=0.8888888889E0
    ac_r=0
    u0=0.
    u1=1.
    du=(u1-u0)/NR
    u=u0-du
    DO iu=1,NR,2 ! Gaussian quadrature
       u=u+2.E0*du
       ac_r=ac_r+W2*dab_reg(u,vp,ib,nni,k2,kb2,betab,mb)
       um=u-du*UPM
       ac_r=ac_r+W13*dab_reg(um,vp,ib,nni,k2,kb2,betab,mb)
       um=u+du*UPM
       ac_r=ac_r+W13*dab_reg(um,vp,ib,nni,k2,kb2,betab,mb)
    ENDDO
    ac_r=ac_r*du
  END SUBROUTINE a_reg
```

3. Quantum Contribution

For the quantum term we make the change of variables $v_{pb} = v_p\, u$ so that

$$\mathcal{A}_b^{\rm QM} = -\frac{e_p^2\,\kappa_b^2}{4\pi}\left(\frac{\beta_b m_b}{2\pi}\right)^{1/2} v_p \int_0^\infty du\left[\mathrm{Re}\,\psi\Big\{1+i\,\frac{\bar\eta_{pb}}{u}\Big\} - \ln\Big\{\frac{\bar\eta_{pb}}{u}\Big\}\right]\frac{1}{\beta_b m_b v_p^2\,u}$$
$$\left[e^{-\frac{1}{2}\,\beta_b m_b v_p^2 (u-1)^2}\left(1-\frac{1}{\beta_b m_b v_p^2\,u}\right) + e^{-\frac{1}{2}\,\beta_b m_b v_p^2 (u+1)^2}\left(1+\frac{1}{\beta_b m_b v_p^2\,u}\right)\right]. \quad \text{(A21)}$$

The quantum function we need to code is therefore

$$\mathcal{A}_b^{\rm QM} = \underbrace{\left[\frac{e_p^2\,\kappa_b^2}{4\pi}\left(\frac{\beta_b m_b}{2\pi}\right)^{1/2} v_p\right]}_{c_{b,1}\cdot c_{b,2}} \cdot \mathsf{A}_1^{\rm QM}(a_{pb},\tilde\eta_{pb})\ , \quad \text{(A22)}$$

where the arguments of the function are defined by

$$a_{pb} = \frac{1}{2}\,\beta_b m_b\, v_p^2 \tag{A23}$$

$$\tilde{\eta}_{pb} = \frac{e_p e_b}{4\pi\hbar v_p} = |Z_p Z_b|\,\frac{e^2}{8\pi a_0}\,\frac{2a_0}{\hbar}\,\frac{1}{v_p} = |Z_p Z_b|\ \cdot 13.606\,\mathrm{eV}\ \cdot \frac{2\cdot 5.29\times 10^{-9}\,\mathrm{cm}}{6.5821\times 10^{-16}\,\mathrm{eV\,s}}\,\frac{1}{v_p}$$

$$= 2.1870\times 10^8\,\frac{|Z_p Z_b|}{v_p\cdot(\mathrm{cm/s})^{-1}}\ , \tag{A24}$$

and the function itself takes the form

$$\mathsf{A}_1^{\mathrm{QM}}(a,\eta) = -\int_0^\infty du\,\left[\mathrm{Re}\,\psi\Big\{1+i\,\frac{\eta}{u}\Big\} - \ln\Big\{\frac{\eta}{u}\Big\}\right] \frac{1}{2a\,u}\left[\Big(e^{-a(u-1)^2}+e^{-a(u+1)^2}\Big) - \frac{e^{-a(u-1)^2}-e^{-a(u+1)^2}}{2a\,u}\right]\ . \tag{A25}$$

acoeff.f90:

```
FUNCTION daq(u, a, eta)
USE physvars
  IMPLICIT NONE
  REAL,                          INTENT(IN)  :: u          ! [dimensionless]
  REAL,                          INTENT(IN)  :: a          ! [dimensionless]
  REAL,                          INTENT(IN)  :: eta        ! [dimensionless]
  REAL                                       :: daq  ! [dimensionless]
  REAL, PARAMETER :: AMAX=25.
  REAL            :: repsi, au, eu, au2, ap, am, psilog, ch, sh
  eu=eta/u
  psilog=repsi(eu) - LOG(eu)
  au =2*a*u
  au2=a*u*u
  IF (a <= AMAX) THEN
    ch =EXP(-au2)*COSH(au)
    sh =EXP(-au2)*SINH(au)
  ELSE
    ap = au-au2-a
    am =-au-au2-a
    ch =0.5*(EXP(ap)+EXP(am))
    sh =0.5*(EXP(ap)-EXP(am))
  ENDIF
  daq=-psilog*2*(ch - sh/au)/au
END FUNCTION daq


SUBROUTINE a_quantum(ib, a, eta, aq)
  IMPLICIT NONE
  INTEGER, INTENT(IN)  :: ib    ! species index
  REAL,    INTENT(IN)  :: a     ! [dimensionless] (1/2) betab mb vp^2
  REAL,    INTENT(IN)  :: eta   ! [dimensionless] ep eb/4pi hbar vp
  REAL,    INTENT(OUT) :: aq
  REAL                 :: u0, u1, du, u, um
  INTEGER, PARAMETER :: NQ=1000           ! integration regions quantum : must
  REAL,    PARAMETER :: UPM=0.7745966692E0 ! parameters for Gaussian Quad
  REAL,    PARAMETER :: W13=0.5555555556E0, W2=0.8888888889E0
  REAL    :: daq
  INTEGER :: iu
  aq=0
  u0=0.
```

```
  aq=0
  IF (ib == 1) THEN
     u0=0
     u1=4./SQRT(a)
  ELSE
     u0=1-10./SQRT(a)
     u0=MAX(0.,u0)
     u1=1+10./SQRT(a)
  ENDIF
  du=(u1-u0)/NQ
  u=u0-du
  DO iu=1,NQ,2 ! Gaussian quadrature
     u=u+2.E0*du
     aq=aq+W2*daq(u,a,eta)
     um=u-du*UPM
     aq=aq+W13*daq(um,a,eta)
     um=u+du*UPM
     aq=aq+W13*daq(um,a,eta)
  ENDDO
  aq=aq*du
END SUBROUTINE a_quantum
```

Appendix B: Complete Source Code Listing: acoeff.f90

This section gives the complete listing for the source acoeff.f90 as it currently stands, including comments for the user and comments that I have made for myself (the latter will eventually disappear). This source module calculates the A-coefficients (coeff_bps), their low energy asymptotic limits (coeff_bps_small_E), and their high energy asymptotic limits (coeff_bps_high_E). For the electron, there are two distinct high energy regions: an intermediate high energy regime $T \ll E_p \ll (m_{\rm I}/m_e)\,T$ and an extreme high energy regime $E \gg (m_{\rm I}/m_e)\,T$.

Note: Currently, the subroutine coeff_bps_high_E only returns the total electron contribution $\mathcal{A}_e$ (regular + singular + quantum).

To do: To complete the subroutine coeff_bps_high_E, I need to calculate the regular and singular contributions for the electrons in both high energy regimes. That is to say, I need to calculate the asymptotic limits of $\mathcal{A}^{\rm C}_{e\,,\,{\rm S}}$ and $\mathcal{A}^{<}_{e\,,\,{\rm R}}$ respectively. The quantum asymptotic correction can then be obtained by

$$\mathcal{A}^{\rm QM}_e = \mathcal{A}_e - \mathcal{A}^{\rm C}_e = \mathcal{A}_e - (\mathcal{A}^{\rm C}_{e\,,\,{\rm S}} + \mathcal{A}^{<}_{e\,,\,{\rm R}}).$$

Before coeff_bps_high_E returns the same quantities for electrons and ions, I will need to analytically calculate $\mathcal{A}^{\rm C}_{e\,,\,{\rm S}}$ and $\mathcal{A}^{<}_{e\,,\,{\rm R}}$ and their high energy limits. To repeat the above note: until I finish this calculation, the subroutine coeff_bps_high_E only returns the total electron contribution $\mathcal{A}_e$, although it returns the complete set of contributions for $\mathcal{A}_{\rm I}$.

1. The A-Coefficients

acoeff.f90:

```
!
! ROUTINE: bps_acoeff_ab_mass(nni, ep, mp, zp, ia, ib, betab, zb, mb, nb, &
!            a_ab, a_ab_sing, a_ab_reg, a_ab_qm)
!
! Assume a plasma composed of several species b, each separately in
! thermal equilibrium with themselves but not necessarily with each
! other[1]. This routine returns several useful components of the
! corresponding A-coefficients introduced in Note [2] below (BPS).
!
! UNITS: A_{pb} has units of [MeV/micron] (subject to change in updates)
!
! THE PHYSICS:
! The various subsystems b will exchange coulomb energy and they will
! eventually equilibrate to a common temperature. The A-coefficients
! introduced in Ref. [2] encode this coulomb energy exchange, exactly to
! leading and next-to-leading orders in the plasma coupling constant g.
```

```
! See Refs. [3,4,5] for more details. For a weakly coupled plasma (g << 1),
! the BPS calculation is essentially exact, and the error is O(g). Physical
! properties of interest, such as the stopping power dE/dx and the temperature
! equilibration rate between plasma species, can be obtained directly from
! the A-coefficients.
!
! USAGE:
! Since electrons are thousands of times lighter than ions, one of the most
! physically accessible regime is the in which the electrons have a temperature
! T_e and the ions have a (possibly different) common temperature T_I. This
! is why the output is organized into electron contributions and total ion
! contributions (sum over all ions).
!
! INPUT: nni, ep, zp, mp, ia, ib, betab, zb, mb, nb
!
! Describe the incident projectile and the background plasma.
!
! projectile input quantities:
! ep : classical kinetic energy of the projectile [keV]
! zp : charge of the projectile in units of Z_p [dimensionless]
! mp : mass of the projectile [keV], i.e. mp = mp[grams]*c^2
!
! plasma input quantities:
! nni  : Number of total plasma species = number ion species + 1
! zb   : Charges of the plasma species. By convention zp(1) is the
!      : electron plasma component. [dimensionless, Array]
! betab: Inverse temperatures of the plasma components. For an
!        electron-ion plasma, set betab(1)=1/T_e and all other
!        values of the array to 1/T_I [keV^-1].
! mb   : Masses of the plasma species [keV].
! nb   : Number densities of the plasma species [cm^-3].
! ia   : First plasma species [usually the projectile]
! ib   : Second plasma species
!
! OUTPUT: a_ab, a_ab_sing, a_ab_reg, a_ab_qm
!
! Each plasma component b makes a linear contribution A_b to the total
! A-coefficient, i.e. A = sum_b A_b [5]. Each A_b in turn can be be
! decomposed into a classical-quantum or electron-ion contributions.
!
! classical electron  : ac_e
! classical ion       : ac_i [sum over all ions]
! classical total     : ac_tot = ac_e + ac_i
! quantum   electron  : aq_e
! quantum   ion       : aq_i [sum over all ions]
! quantum   total     : a_tot = aq_e + aq_i
! total     electric  : a_e = ac_e + aq_e
! total     ion       : a_i = ac_i + aq_i
! total               ! a_tot = a_e + a_i
!
! NOTES:
! [1] The temperatures T_b may therefore all differ. By convention
!     I take b=1 for the electron component of the plasma. A very
!     useful and interesting parameter regime is the one in which
!     the ions have a common temperature T_I and the electron have
!     a temperature T_e, usually with T_e =/= T_I.  See also USAGE
!     and note [3] below.
!
! [2] BPS paper
!     L. Brown, D. Preston, and R. Singleton~Jr.,
!     "Charged Particle Motion in a Highly Ionized Plasma",
!     Physics Reports, 410 (2005) 237
!     [arXiv:physics/0501084]
!
```

```
! [3] The code employs rationalized cgs units in which the dimensionless
!     plasma coupling parameter is defined by g = e^2 kappa/(4Pi*T); in
!     these units the Debye wavenumber is determined by kappa^2 = e^2 n/T
!     and the plasma frequency by omega^2 = e^2 n/m. A weakly coupled
!     plasma is one for which g << 1, i.e. a plasma with thermal kinetic
!     energy (of order the temperature T) dominates the coulomb potential
!     energy (for particles separated by a Debye length). In the more
!     common non-rationalized cgs units, we define g = e^2 kappa/T, with
!     kappa^2 = 4 Pi e^2 n/T and omega^2 = 4 Pi e^2 n/m.
!
! [4] For coulomb energy exchange processes, the leading and next-to-
!     leading order terms in the plasma coupling g are proportional to
!     g^2*ln(g) and g^2, respectively. That is to say, for a property
!     denoted by F, one can expand F in powers of g in the form:
!
!       F(g,eta) = A(eta)*g^2*ln(g) + B(eta)*g^2 + O(g^3)
!                = A(eta)*g^2*[ ln(C(eta)*g)+O(g) ],
!
!     where eta is the dimensionless quantum parameter (eta <<1 means
!     extreme classical scattering while eta >>1 means the extreme quantum
!     limit). The relative error of BPS is therefore O(g). At the center of
!     the sun g=0.4, and so the error of Ref. [1] is only of order 4% in
!     this case. For the processes of charged stopping power and electron-
!     ion temperature equilibration, Ref. [1] calculates the corresponding
!     functions A(eta) and B(eta) exactly, including all orders in the
!     two-body quantum scattering parameter eta = e^2/4Pi*hbar*v_thermal
!     (this means that BPS gives the correct interpolation between the
!     classical and quantum regimes, exact to leading and next-to-leading
!     order). The O(g^3) terms physically correspond to 3-body correlations
!     within the plasma, and for a sufficiently weak plasma these are
!     negligible. For strongly coupled plasmas (g >> 1), all terms in a
!     g-expansion are important and the BPS calculation is not applicable.
!
! [5] It makes sense to talk about separate linear contribution A_b
!     contributing *from* a given plasma component b only for a weakly
!     coupled plasma. More exactly, A=sum_b A_b holds true only up to
!     leading and next-to-leading order in the plasma coupling g. This is
!     the order to which Ref. [2] calculates all quantities, and therefore
!     BPS works to a consistent order in g.
!
!
! vp = projectile speed [cm/s]
!
!            [ 2 Ep ]
!    = c sqrt[ ---- ]  where mp and Ep are in keV and
!            [ mpc2 ]  c is the speed of light in cm/s
!
!
!         ep^2 kb^2
! c1   =  --------- = 2 zp**2 * Be * kb^2 * a0  [keV/cm]
!            4 Pi                              [MeV/micron]
!
!        [ betab mbc2 ]^1/2
! c2 =   |------------ |       vp   [dimensionless]
!        [    2 Pi     ]
!
! where
!           e^2
! Be   =  --------- = 13.606E-3   [keV]
!         8 Pi a0                Bohr radius: a0=5.29E-9 cm
!
!
!
!
```

```
!%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
! main driver for A-coefficient for general quantum and electron-mass regimes
!%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
!
      SUBROUTINE bps_acoeff_ab_mass(nni, ep, mp, zp, ia, ib, betab, zb, mb, nb, &
            a_ab, a_ab_sing, a_ab_reg, a_ab_qm)
      USE physvars
      USE mathvars
        IMPLICIT NONE                                                  ! Plasma:
        INTEGER,                              INTENT(IN)  :: nni       !  number of ions
        REAL,                                 INTENT(IN)  :: ep        !  energy input [ke
        REAL,                                 INTENT(IN)  :: mp        !  mass [keV]
        REAL,                                 INTENT(IN)  :: zp        !  charge
        INTEGER,                              INTENT(IN)  :: ia        !
        INTEGER,                              INTENT(IN)  :: ib        !
        REAL,    DIMENSION(1:nni+1),          INTENT(IN)  :: betab     !  temp array [1/ke
        REAL,    DIMENSION(1:nni+1),          INTENT(IN)  :: mb        !  mass array [keV]
        REAL,    DIMENSION(1:nni+1),          INTENT(IN)  :: nb        !  density [1/cc]
        REAL,    DIMENSION(1:nni+1),          INTENT(IN)  :: zb        !  charge array
                                                                       !
                                                                       ! A-coeffs [MeV/mic
        REAL,                                 INTENT(OUT) :: a_ab
        REAL,                                 INTENT(OUT) :: a_ab_sing
        REAL,                                 INTENT(OUT) :: a_ab_reg
        REAL,                                 INTENT(OUT) :: a_ab_qm

        REAL,    DIMENSION(1:nni+1)  :: mpb, mbpb, kb2, ab
        REAL                         :: vp, zp2, k, k2, kd, kd2, a, b, eta
        REAL                         :: ac_r, ac_s, aq, c1, c2

        REAL, PARAMETER              :: EPS_SMALL_E=2.E-4
        REAL, PARAMETER              :: EPS_SMALL_E_SING=2.E-4
        REAL, PARAMETER              :: EPS_SMALL_E_REG=2.E-4
!
! initialize components of A-coefficients
!
        kb2=8*PI*AOCM*BEKEV*zb*zb*nb*betab
        kd2 = SUM(kb2)                ! [1/cm^2]
        kd  = SQRT(kd2)               ! [1/cm]
        k2  = kb2(1)                  ! [1/cm^2]
        k   = SQRT(k2)                ! [1/cm]   k = k_e
!
! Loop over charged plasma species
!
        mpb = mp*mb/(mp+mb)            ! [keV]
        mbpb= mb/mpb                   ! [dimensionless]
        vp =CC*SQRT(2*ep/mp)           ! [cm/s]
        zp2=zp**2                      ! [dimensionless]
                                       ! ab=(1/2) betab(ib)*mbc2(ib)*vp2/CC2
        ab  =0.5*betab*mb*vp*vp/CC2    ! [dimensionless]
        IF (zb(ib) .NE. 0.) THEN
        a  =ab(ib)
        b  =-Log(2*betab(ib)*BEKEV*ABS(zp*zb(ib))*k*AOCM*mbpb(ib) )-2*GAMMA+2
        eta=ABS(zp*zb(ib))*2.1870E8/vp ! defined with projectile velocity vp
        c1=2*zp2*BEKEV*kb2(ib)*AOCM    ! [keV/cm] c1 = e_p^2 kappa_b^2/(4 Pi)
        c1=c1*1.E-7                    ! [MeV/micron]
        c2=SQRT(a/PI)                  ! [dimensionless]
                                       ! c2=SQRT(betab(ib)*mb(ib)/TWOPI)*vp/CC
!
! A_{ab}-classical-singular
!
        CALL a_sing_mass(a,b,ac_s)
        a_ab_sing=c1*c2*ac_s
!
```

```
! A_{ab}-classical-regular
!
        CALL a_reg_mass(nni,ia,ib,vp,k2,kb2,betab,mb,ac_r)
        a_ab_reg=c1*ac_r
!
! A_{ab}-quantum
!
        CALL a_quantum_mass(ia,ib,a,eta,aq) ! eta = dimensionless quantum param.
        a_ab_qm=c1*c2*aq
!
! A_{ab}-total
!
        a_ab=a_ab_sing + a_ab_reg + a_ab_qm
        ENDIF
      END SUBROUTINE bps_acoeff_ab_mass
!
!%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
! Assembles the matrix A_{ab} of the A-coefficients.
!%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
!
      SUBROUTINE bps_acoeff_ab_matrix(nni, ep, betab, zb, mb, nb,    &
        a_ab, a_ab_sing, a_ab_reg, a_ab_qm, a_tot, a_i, a_e, ac_tot, &
        ac_i, ac_e, aq_tot, aq_i, aq_e, ac_s_i, ac_s_e, ac_r_i, ac_r_e)
      USE physvars
      USE mathvars
        IMPLICIT NONE                                           ! Plasma:
        INTEGER,                            INTENT(IN)  :: nni    !  number of ions
        REAL,                               INTENT(IN)  :: ep     !  energy
        REAL,    DIMENSION(1:nni+1),        INTENT(IN)  :: betab  !  temp array [1/ke
        REAL,    DIMENSION(1:nni+1),        INTENT(IN)  :: zb     !  charge array
        REAL,    DIMENSION(1:nni+1),        INTENT(IN)  :: mb     !  mass array [keV]
        REAL,    DIMENSION(1:nni+1),        INTENT(IN)  :: nb     !  density [1/cc]
                                                                !
                                                                ! A-coeffs [MeV/mic
        REAL,    DIMENSION(1:nni+1,1:nni+1),INTENT(OUT) :: a_ab
        REAL,    DIMENSION(1:nni+1,1:nni+1),INTENT(OUT) :: a_ab_sing
        REAL,    DIMENSION(1:nni+1,1:nni+1),INTENT(OUT) :: a_ab_reg
        REAL,    DIMENSION(1:nni+1,1:nni+1),INTENT(OUT) :: a_ab_qm
        REAL,    DIMENSION(1:nni+1),        INTENT(OUT) :: a_tot
        REAL,    DIMENSION(1:nni+1),        INTENT(OUT) :: a_i
        REAL,    DIMENSION(1:nni+1),        INTENT(OUT) :: a_e
        REAL,    DIMENSION(1:nni+1),        INTENT(OUT) :: ac_tot
        REAL,    DIMENSION(1:nni+1),        INTENT(OUT) :: ac_i
        REAL,    DIMENSION(1:nni+1),        INTENT(OUT) :: ac_e
        REAL,    DIMENSION(1:nni+1),        INTENT(OUT) :: aq_tot
        REAL,    DIMENSION(1:nni+1),        INTENT(OUT) :: aq_i
        REAL,    DIMENSION(1:nni+1),        INTENT(OUT) :: aq_e
        REAL,    DIMENSION(1:nni+1),        INTENT(OUT) :: ac_s_i
        REAL,    DIMENSION(1:nni+1),        INTENT(OUT) :: ac_s_e
        REAL,    DIMENSION(1:nni+1),        INTENT(OUT) :: ac_r_i
        REAL,    DIMENSION(1:nni+1),        INTENT(OUT) :: ac_r_e

        REAL    :: aab, aab_sing, aab_reg, aab_qm
        REAL    :: mp, zp
        INTEGER :: ia, ib

        a_i   = 0
        ac_s_i= 0
        ac_r_i= 0
        ac_i  = 0
        aq_i  = 0
        DO ia=1,nni+1
          mp=mb(ia)
          zp=zb(ia)
          DO ib=1,nni+1
            CALL bps_acoeff_ab_mass(nni, ep, mp, zp, ia, ib, betab, zb, mb, nb, &
```

```
            aab, aab_sing, aab_reg, aab_qm)
            a_ab(ia,ib)     =aab
            a_ab_sing(ia,ib)=aab_sing
            a_ab_reg(ia,ib) =aab_reg
            a_ab_qm(ia,ib)  =aab_qm
            IF (ib == 1) THEN
               a_e(ia)   = aab
               ac_s_e(ia)= aab_sing
               ac_r_e(ia)= aab_reg
               ac_e(ia)  = aab_sing + aab_reg
               aq_e(ia)  = aab_qm
            ELSE
               a_i(ia)   = a_i(ia)    + aab
               ac_s_i(ia)= ac_s_i(ia) + aab_sing
               ac_r_i(ia)= ac_r_i(ia) + aab_reg
               ac_i(ia)  = ac_i(ia)   + aab_sing + aab_reg
               aq_i(ia)  = aq_i(ia)   + aab_qm
            ENDIF
          ENDDO
          a_tot(ia) = a_e(ia)  + a_i(ia)
          ac_tot(ia)= ac_e(ia) + ac_i(ia)
          aq_tot(ia)= aq_e(ia) + aq_i(ia)
        ENDDO
      END SUBROUTINE bps_acoeff_ab_matrix
!
!%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
! Returns A_{p I} = \sum_i A_{p i} for backward compatibility
!%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
!
      SUBROUTINE bps_acoeff_ei_mass(nni, ep, zp, mp, betab, zb, mb, nb, &
            a_tot, a_i, a_e, ac_tot, ac_i, ac_e, aq_tot, aq_i, aq_e,&
            ac_s_i, ac_s_e, ac_r_i, ac_r_e)
      USE physvars
      USE mathvars
      USE controlvars
        IMPLICIT NONE                                          ! Plasma:
        INTEGER,                          INTENT(IN)  :: nni   !  number of ions
        REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: betab  !  temp array [1/keV]
        REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: mb     !  mass array [keV]
        REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: nb     !  density [1/cc]
        REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: zb     !  charge array
                                                           !
                                                           ! Projectile
        REAL,                             INTENT(IN)  :: ep    !  projectile energy [keV]
        REAL,                             INTENT(IN)  :: mp    !  projectile mass   [keV]
        REAL,                             INTENT(IN)  :: zp    !  projectile charge
                                                           !
                                                           ! A-coeffs [MeV/micron]
        REAL,                             INTENT(OUT) :: a_tot  !  electron + ion
        REAL,                             INTENT(OUT) :: a_i    !  ion contribution
        REAL,                             INTENT(OUT) :: a_e    !  electron contribution
        REAL,                             INTENT(OUT) :: ac_tot !  classical
        REAL,                             INTENT(OUT) :: ac_i   !  classical
        REAL,                             INTENT(OUT) :: ac_e   !  classical
        REAL,                             INTENT(OUT) :: aq_tot !  quantum
        REAL,                             INTENT(OUT) :: aq_i   !  quantum
        REAL,                             INTENT(OUT) :: aq_e   !  quantum
        REAL,                             INTENT(OUT) :: ac_s_i
        REAL,                             INTENT(OUT) :: ac_s_e
        REAL,                             INTENT(OUT) :: ac_r_i
        REAL,                             INTENT(OUT) :: ac_r_e

        REAL     :: adum, ac_s, ac_r, aq
        INTEGER  :: ia, ib, nnb
```

```
!
! initialize components of A-coefficients
!
        a_tot =0  ! electron + ion
        a_i   =0  ! ion contribution
        a_e   =0  ! electron contribution
        ac_tot=0  ! classical total
        ac_e  =0  ! classical electron
        ac_i  =0  ! classical ion
        aq_tot=0  ! quantum total
        aq_e  =0  ! quantum electron
        aq_i  =0  ! quantum ion
        ac_s_i=0
        ac_s_e=0
        ac_r_i=0
        ac_r_e=0

        NNB = nni+1                 ! number of ions + electrons
        ia=1
        DO ib=1,nni+1
        IF (zb(ib) .NE. 0.) THEN
            CALL bps_acoeff_ab_mass(nni, ep, mp, zp, ia, ib, betab, zb, mb, nb, &
            adum, ac_s, ac_r, aq)
            CALL x_collect(ib, NNB, ac_s, ac_r, aq,       &
            a_tot, a_i, a_e, ac_tot, ac_i, ac_e, aq_tot,  &
            aq_i, aq_e, ac_s_i, ac_s_e, ac_r_i, ac_r_e)
        ENDIF
        ENDDO
      END SUBROUTINE bps_acoeff_ei_mass
!
!%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
! singular contribution for non-zero electron mass
!%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
!
      SUBROUTINE a_sing_mass(a, b, ac_s)
        REAL,    INTENT(IN)  :: a
        REAL,    INTENT(IN)  :: b
        REAL,    INTENT(OUT) :: ac_s
        REAL                 :: u0, u1, du, u, um
        INTEGER, PARAMETER :: NS=1000 ! integration regions: must be even
        REAL,    PARAMETER :: UPM=0.7745966692E0 ! parameters for Gaussian Quad
        REAL,    PARAMETER :: W13=0.5555555556E0, W2=0.8888888889E0
           ac_s=0
           u0=0
           u1=1
           du=(u1-u0)/NS
           u=u0-du
           DO iu=1,NS,2 ! Gaussian quadrature
              u=u+2.E0*du
              ac_s=ac_s+W2*dab_sing(u,a,b)
              um=u-du*UPM
              ac_s=ac_s+W13*dab_sing(um,a,b)
              um=u+du*UPM
              ac_s=ac_s+W13*dab_sing(um,a,b)
           ENDDO
           ac_s=ac_s*du
      END SUBROUTINE a_sing_mass
!
      FUNCTION dab_sing(u, a, b)
        IMPLICIT NONE
        REAL,         INTENT(IN)  :: u        ! [dimensionless]
        REAL,         INTENT(IN)  :: a        ! [dimensionless]
                                              ! a=(1/2)*beta*mpc2*vp^2/C^2
        REAL,         INTENT(IN)  :: b        ! [dimensionless]
        REAL                      :: dab_sing ! [dimensionless]
        dab_sing=SQRT(u)*EXP(-a*u)*(-LOG(u/(1-u)) + b)
      END FUNCTION dab_sing
```

```
!
!%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
! regular contribution for non-zero electron mass
!%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
!
      FUNCTION dab_reg(u, vp, ia, ib, nni, k2, kb2, betab, mb)
      USE mathvars
      USE physvars
        IMPLICIT NONE
        REAL,                          INTENT(IN)  :: u      ! [dimensionless]
        REAL,                          INTENT(IN)  :: vp     ! Projectile velocity [cm/
        INTEGER,                       INTENT(IN)  :: ia     ! Species number
        INTEGER,                       INTENT(IN)  :: ib     ! Species number
        INTEGER,                       INTENT(IN)  :: nni    ! Number of ion species
        REAL,                          INTENT(IN)  :: k2     ! Wave-number squared [1/c
        REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: kb2    ! Debye wavenumber squared
        REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: betab  ! Temperature array [1/keV
        REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: mb     ! Mass array [keV]
        REAL                                     :: dab_reg! [dimensionless]
        REAL,    DIMENSION(1:nni+1) :: kbar2b, ab, ab2
        REAL                        :: fr, fi, fabs, farg, h, r_ib
        REAL                        :: kcb, bm_ic, bm_ib, a_ic, a_ib, ex, au
        INTEGER                     :: ic
        ab=SQRT(0.5*betab*mb)*vp/CC
        ab2=ab*ab
        kbar2b=kb2/k2
        CALL frfi(u,nni,kbar2b,ab,fr,fi,fabs,farg)
        h=2*(fr*farg + fi*LOG(fabs))*u

!
! construct spectral weight ratio Rb=rho_b/rho_tot
!
!*!
!         r_ib=0
!         DO ic=1,nni+1
!           r_ib=r_ib + kbar2b(ib)*(ab(ic)/ab(ib))*EXP((ab2(ib)-ab2(ic))*u*u)
!         ENDDO
!         r_ib=1./r_ib
!*!
        r_ib=0
        bm_ib=betab(ib)*mb(ib)
        a_ib =ab(ib)*ab(ib)
        DO ic=1,nni+1
           kcb=kb2(ic)/k2
           bm_ic=betab(ic)*mb(ic)
           a_ic =ab(ic)*ab(ic)
           IF (ic == ib) THEN
              ex=1.
           ELSE
              au=(a_ic-a_ib)*u
              ex=EXP(-au)
           ENDIF
           r_ib=r_ib + kcb*SQRT(bm_ic/bm_ib)*ex
        ENDDO
        r_ib=1./r_ib
!*!
!r_ib=1.
!*!
!
        dab_reg=-r_ib*h/TWOPI
      END FUNCTION dab_reg

      SUBROUTINE a_reg_mass(nni, ia, ib, vp, k2, kb2, betab, mb, ac_r)
      USE physvars
        IMPLICIT NONE
        INTEGER,                       INTENT(IN)  :: nni
```

```
        INTEGER,                        INTENT(IN)  :: ia
        INTEGER,                        INTENT(IN)  :: ib
        REAL,                           INTENT(IN)  :: vp
        REAL,                           INTENT(IN)  :: k2
        REAL,                           INTENT(IN)  :: kb2
        REAL,    DIMENSION(1:nni+1),    INTENT(IN)  :: betab
        REAL,    DIMENSION(1:nni+1),    INTENT(IN)  :: mb
        REAL,                           INTENT(OUT) :: ac_r
        REAL,    DIMENSION(1:nni+1)     :: ab
!       INTEGER, PARAMETER :: NR=10 ! integration regions: must be even
        INTEGER, PARAMETER :: NR=100 ! integration regions: must be even
        REAL,    PARAMETER :: UPM=0.7745966692E0 ! parameters for Gaussian Quad
        REAL,    PARAMETER :: W13=0.5555555556E0, W2=0.8888888889E0
        REAL               :: u0, u1, du, u, um, dab_reg
        INTEGER            :: iu
        ab=SQRT(0.5*betab*mb)*vp/CC
        ac_r=0
        u0=0.0
        u1=1.
!       u1=MIN(1.,5/(ab(ib)**2)) ! support can lie << 1
        du=(u1-u0)/NR
        u=u0-du
        DO iu=1,NR,2 ! Gaussian quadrature
           u=u+2.*du
           ac_r=ac_r+W2*dab_reg(u,vp,ia,ib,nni,k2,kb2,betab,mb)
           um=u-du*UPM
           ac_r=ac_r+W13*dab_reg(um,vp,ia,ib,nni,k2,kb2,betab,mb)
           um=u+du*UPM
           ac_r=ac_r+W13*dab_reg(um,vp,ia,ib,nni,k2,kb2,betab,mb)
        ENDDO
        ac_r=ac_r*du
!*!
!        um=1
!        ac_r=dab_reg(um,vp,ia,ib,nni,k2,kb2,betab,mb)
!*!
      END SUBROUTINE a_reg_mass
!
!%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
! quantum contribution for non-zero electron mass
!%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
!
      FUNCTION daq(u, a, eta)
      USE physvars
        IMPLICIT NONE
        REAL,                           INTENT(IN)  :: u          ! [dimensionless]
        REAL,                           INTENT(IN)  :: a          ! [dimensionless]
        REAL,                           INTENT(IN)  :: eta        ! [dimensionless]
        REAL                                        :: daq  ! [dimensionless]
        REAL            :: repsi, au, eu, au2, ap, am, psilog, ch, sh, csh
        eu=eta/u
        psilog=repsi(eu) - LOG(eu)
        au =2*a*u
        au2=a*u*u
        ap = au-au2-a
        am =-au-au2-a
        ch =0.5*(EXP(ap)+EXP(am))
        sh =0.5*(EXP(ap)-EXP(am))
        csh=2*(ch - sh/au)/au
        daq=-psilog*csh
      END FUNCTION daq

      SUBROUTINE a_quantum_mass(ia, ib, a, eta, aq)
        IMPLICIT NONE
        INTEGER, INTENT(IN)  :: ia    ! species index
        INTEGER, INTENT(IN)  :: ib    ! species index
        REAL,    INTENT(IN)  :: a     ! [dimensionless] (1/2) betab mb vp^2
```

```
        REAL,    INTENT(IN)  :: eta   ! [dimensionless] ep eb/4pi hbar vp
        REAL,    INTENT(OUT) :: aq
        REAL                 :: u0, u1, du, u, um
        INTEGER, PARAMETER :: NQ=1000            ! integration regions quantum : must
        REAL,    PARAMETER :: UPM=0.7745966692E0 ! parameters for Gaussian Quad
        REAL,    PARAMETER :: W13=0.5555555556E0, W2=0.8888888889E0
        REAL    :: daq
        INTEGER :: iu
        aq=0
        u0=0.
        aq=0
        IF (ib == ia) THEN
           u0=0
           u1=4./SQRT(a)
        ELSE
           u0=1-10./SQRT(a)
           u0=MAX(0.,u0)
           u1=1+10./SQRT(a)
        ENDIF
        du=(u1-u0)/NQ
        u=u0-du
        DO iu=1,NQ,2 ! Gaussian quadrature
           u=u+2.E0*du
           aq=aq+W2*daq(u,a,eta)
           um=u-du*UPM
           aq=aq+W13*daq(um,a,eta)
           um=u+du*UPM
           aq=aq+W13*daq(um,a,eta)
        ENDDO
        aq=aq*du
      END SUBROUTINE a_quantum_mass
!
!
!=============== dE/dx from A-coefficient ================================
!
!
! This is a driver to check the analytic evalulation dE_b/dx
! against the one obtained by differentiating A_b.
!
!
! dE_b        [            1                  d                          ]
! ----(vp) =  [ 1  -  ------------- Sum_l -------  {\hat vp}^l A_b(vp)  ]
!  dx         [        beta_b mp vp       d vp^l                        ]
!
!
!            [           2 T_b   ]                 T_b     dA_b
!         =  [ 1  -  ---------- ] * A_b(vp) -  ------- * ----(vp)
!            [         mp vp^2  ]                mp vp     dvp
!
!            [       T_b  ]                     dA_b
!         =  [ 1  -  ---- ] * A_b(Ep) -  T_b * ----(Ep)
!            [        Ep  ]                     dEp
!
!
      SUBROUTINE acoeff_dedx_bps(nni,ep,zp,mp,betab,zb,mb,nb,  &
            dedx_a_tot, dedx_a_i, dedx_a_e, dedxc_a_tot, dedxc_a_i, dedxc_a_e, &
            dedxq_a_tot, dedxq_a_i, dedxq_a_e, dedxc_a_s_i, dedxc_a_s_e,       &
            dedxc_a_r_i, dedxc_a_r_e)
      USE physvars
      USE mathvars
        IMPLICIT NONE                                      ! Plasma:
        INTEGER,                       INTENT(IN)  :: nni    !  number of ions
        REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: betab  !  temp array [1/keV]
        REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: mb     !  mass array [keV]
        REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: nb     !  density [1/cc]
        REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: zb     !  charge array
```

```
                                                !
                                                ! Projectile
REAL,                          INTENT(IN)  :: ep     !  projectile energy [keV]
REAL,                          INTENT(IN)  :: mp     !  projectile mass   [keV]
REAL,                          INTENT(IN)  :: zp     !  projectile charge
                                                !
                                                     ! dE/dx [MeV/micron]
REAL,                          INTENT(OUT) :: dedx_a_tot  !  electron + ion
REAL,                          INTENT(OUT) :: dedx_a_i    !  ion contribution
REAL,                          INTENT(OUT) :: dedx_a_e    !  electron contribut
REAL,                          INTENT(OUT) :: dedxc_a_tot !  classical
REAL,                          INTENT(OUT) :: dedxc_a_i   !  classical
REAL,                          INTENT(OUT) :: dedxc_a_e   !  classical
REAL,                          INTENT(OUT) :: dedxq_a_tot !  quantum
REAL,                          INTENT(OUT) :: dedxq_a_i   !  quantum
REAL,                          INTENT(OUT) :: dedxq_a_e   !  quantum
REAL,                          INTENT(OUT) :: dedxc_a_s_i
REAL,                          INTENT(OUT) :: dedxc_a_s_e
REAL,                          INTENT(OUT) :: dedxc_a_r_i
REAL,                          INTENT(OUT) :: dedxc_a_r_e

REAL :: a_tot_p, a_i_p, a_e_p, ac_tot_p, ac_i_p, ac_e_p, aq_tot_p, aq_i_p, aq
REAL :: ac_s_i_p, ac_s_e_p, ac_r_i_p, ac_r_e_p
REAL :: a_tot_m, a_i_m, a_e_m, ac_tot_m, ac_i_m, ac_e_m, aq_tot_m, aq_i_m, aq
REAL :: ac_s_i_m, ac_s_e_m, ac_r_i_m, ac_r_e_m
REAL :: a_tot,   a_i,   a_e,   ac_tot,   ac_i,   ac_e,   aq_tot,   aq_i,   aq
REAL :: ac_s_i,ac_s_e, ac_r_i,ac_r_e
REAL :: te, ti, dep, dep2, epp, epm

te  =1./betab(1)
ti  =1./betab(2)

dedx_a_tot  = 0 ! electron + ion
dedx_a_i    = 0 ! ion contribution
dedx_a_e    = 0 ! electron contribution
dedxc_a_tot = 0 ! classical
dedxc_a_i   = 0 ! classical
dedxc_a_e   = 0 ! classical
dedxq_a_tot = 0 ! quantum
dedxq_a_i   = 0 ! quantum
dedxq_a_e   = 0 ! quantum
dedxc_a_s_i = 0
dedxc_a_s_e = 0
dedxc_a_r_i = 0
dedxc_a_r_e = 0

dep = ep * 1.E-4
dep2 = 2 * dep
CALL bps_acoeff_ei_mass(nni,ep,zp,mp,betab,zb,mb,nb,a_tot,a_i, &
  a_e,ac_tot,ac_i,ac_e,aq_tot,aq_i,aq_e,ac_s_i,ac_s_e,&
  ac_r_i,ac_r_e)

epp = ep + dep
CALL bps_acoeff_ei_mass(nni,epp,zp,mp,betab,zb,mb,nb,a_tot_p,a_i_p, &
  a_e_p,ac_tot_p,ac_i_p,ac_e_p,aq_tot_p,aq_i_p,aq_e_p,ac_s_i_p,ac_s_e_p,&
  ac_r_i_p,ac_r_e_p)

epm = ep - dep
CALL bps_acoeff_ei_mass(nni,epm,zp,mp,betab,zb,mb,nb,a_tot_m,a_i_m, &
  a_e_m,ac_tot_m,ac_i_m,ac_e_m,aq_tot_m,aq_i_m,aq_e_m,ac_s_i_m,ac_s_e_m,&
  ac_r_i_m,ac_r_e_m)

dedx_a_tot = (1 - te/ep)*a_tot  - te*(a_tot_p - a_tot_m)/dep2
dedx_a_i = (1 - ti/ep)*a_i - ti*(a_i_p - a_i_m)/dep2
dedx_a_e = (1 - te/ep)*a_e - te*(a_e_p - a_e_m)/dep2
```

```
        dedxq_a_tot= (1 - te/ep)*aq_tot - te*(aq_tot_p-aq_tot_m)/(2*dep)
        dedxq_a_i  = (1 - ti/ep)*aq_i   - ti*(aq_i_p  -aq_i_m)/dep2
        dedxq_a_e  = (1 - te/ep)*aq_e   - te*(aq_e_p  -aq_e_m)/dep2

        dedxc_a_tot= (1 - te/ep)*ac_tot - te*(ac_tot_p-ac_tot_m)/(2*dep)
        dedxc_a_i  = (1 - ti/ep)*ac_i   - ti*(ac_i_p  -ac_i_m)/dep2
        dedxc_a_e  = (1 - te/ep)*ac_e   - te*(ac_e_p  -ac_e_m)/dep2

        dedxc_a_s_i = (1 - te/ep)*ac_s_i   - te*(ac_s_i_p  -ac_s_i_m)/dep2
        dedxc_a_s_e = (1 - te/ep)*ac_s_e   - te*(ac_s_e_p  -ac_s_e_m)/dep2
        dedxc_a_r_i = (1 - te/ep)*ac_r_i   - te*(ac_r_i_p  -ac_r_i_m)/dep2
        dedxc_a_r_e = (1 - te/ep)*ac_r_e   - te*(ac_r_e_p  -ac_r_e_m)/dep2

      END SUBROUTINE acoeff_dedx_bps
!

      SUBROUTINE a_collect(ib, ibmax, ac_s, ac_r, aq, a_tot, a_i, a_e, &
        ac_tot, ac_i, ac_e, aq_tot, aq_i, aq_e, ac_s_i, ac_s_e, ac_r_i, ac_r_e)
        IMPLICIT NONE
        INTEGER, INTENT(IN)    :: ib     ! species index
        INTEGER, INTENT(IN)    :: ibmax  ! species index maximum = NNB+1
        REAL,    INTENT(IN)    :: ac_s   ! singular contribution
        REAL,    INTENT(IN)    :: ac_r   ! regular  contribution
        REAL,    INTENT(IN)    :: aq     ! quantum  contribution
                                         !
        REAL,    INTENT(INOUT) :: a_tot  ! running total over ions
        REAL,    INTENT(INOUT) :: a_i    ! running total over ions
        REAL,    INTENT(INOUT) :: a_e    ! electron component
        REAL,    INTENT(INOUT) :: ac_tot ! running total over ions
        REAL,    INTENT(INOUT) :: ac_i   ! running total over ions
        REAL,    INTENT(INOUT) :: ac_e   ! electron component
        REAL,    INTENT(INOUT) :: aq_tot ! running total over ions
        REAL,    INTENT(INOUT) :: aq_i   ! running total over ions
        REAL,    INTENT(INOUT) :: aq_e   ! electron component
        REAL,    INTENT(INOUT) :: ac_s_i
        REAL,    INTENT(INOUT) :: ac_s_e
        REAL,    INTENT(INOUT) :: ac_r_i
        REAL,    INTENT(INOUT) :: ac_r_e
        REAL :: ac_sr
        ac_sr=ac_s + ac_r
        IF (ib==1) THEN
           ac_e=ac_sr
           aq_e=aq
           a_e =ac_e + aq_e

           ac_s_e=ac_s
           ac_r_e=ac_r
        ELSE
           ac_i=ac_i + ac_sr
           aq_i=aq_i + aq
           a_i =a_i  + ac_sr + aq

           ac_s_i=ac_s_i + ac_s
           ac_r_i=ac_r_i + ac_r
        ENDIF
        IF (ib==ibmax) THEN
           ac_tot = ac_e + ac_i
           aq_tot = aq_e + aq_i
           a_tot  = ac_tot  + aq_tot
        ENDIF
      END SUBROUTINE a_collect
```

2. Low Energy Asymptotics

acoeff.f90 cont.:

```
!
! ROUTINE: SUBROUTINE coeff_bps_small_E(nni, ep, zp, mp, betab, zb, mb, nb, &
!   a_tot_lim, a_i_lim, a_e_lim, ac_tot_lim, ac_i_lim, ac_e_lim, aq_tot_lim,&
!   aq_i_lim, aq_e_lim)
!
! The asymptotic low energy regime E_p << T: this routine returns several
! useful components of the corresponding A-coefficients in the low energy
! regime.
!
! UNITS: A_b has units of [MeV/micron] (subject to change in updates)
!
! The incident projectile and the background plasma.
!
! projectile input quantities:
! ep : classical kinetic energy of the projectile [keV]
! zp : charge of the projectile in units of Z_p [dimensionless]
! mp : mass of the projectile [keV], i.e. mp = mp[grams]*c^2
!
! plasma input quantities:
! nni  : Number of total plasma species = number ion species + 1
! zb   : Charges of the plasma species. By convention zp(1) is the
!      : electron plasma component. [dimensionless, Array]
! betab: Inverse temperatures of the plasma components. For an
!        electron-ion plasma, set betab(1)=1/T_e and all other
!        values of the array to 1/T_I.
! mb   : Masses of the plasma species [keV].
! nb   : Number densities of the plasma species [cm^-3].
!
! OUTPUT: a_tot_lim, a_i_lim, a_e_lim, ac_tot_lim, ac_i+lim, ac_e_lim,
!         aq_tot_lim, aq_i_lim, aq_e_lim
!
! classical electron  : ac_e_lim
! classical ion       : ac_i_lim [sum over all ions]
! classical total     : ac_tot_lim = ac_e_lim + ac_i_lim
! quantum   electron  : aq_e_lim
! quantum   ion       : aq_i_lim [sum over all ions]
! quantum   total     : a_tot_lim = aq_e_lim + aq_i_lim
! total     electric  : a_e_lim = ac_e_lim + aq_e_lim
! total     ion       : a_i_lim = ac_i_lim + aq_i_lim
! total               ! a_tot_lim = a_e_lim + a_i_lim
!
```

```
      SUBROUTINE coeff_bps_small_E(nni, ep, zp, mp, betab, zb, mb, nb,   &
            a_tot_lim, a_i_lim, a_e_lim, ac_tot_lim, ac_i_lim, ac_e_lim, &
            aq_tot_lim, aq_i_lim, aq_e_lim)
      USE physvars
      USE mathvars
        IMPLICIT NONE
        INTEGER,                        INTENT(IN)  :: nni    !  number of ions
        REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: betab  !  temp array [1/keV]
        REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: mb     !  mass array [keV]
        REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: nb     !  density [1/cc]
        REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: zb     !  charge array
                                                           !
                                                 ! Projectile
```

```
        REAL,                          INTENT(IN)  :: ep!  projectile energy [keV]
        REAL,                          INTENT(IN)  :: mp!  projectile mass   [keV]
        REAL,                          INTENT(IN)  :: zp!  projectile charge
                                                           !
                                                           ! A-coeffs [MeV/micron]
        REAL,                          INTENT(OUT) :: a_tot_lim !  electron + ion
        REAL,                          INTENT(OUT) :: a_i_lim   !  ion contribution
        REAL,                          INTENT(OUT) :: a_e_lim   !  electron contributio
        REAL,                          INTENT(OUT) :: ac_tot_lim!  classical
        REAL,                          INTENT(OUT) :: ac_i_lim  !  classical
        REAL,                          INTENT(OUT) :: ac_e_lim  !  classical
        REAL,                          INTENT(OUT) :: aq_tot_lim!  quantum
        REAL,                          INTENT(OUT) :: aq_i_lim  !  quantum
        REAL,                          INTENT(OUT) :: aq_e_lim  !  quantum

        REAL    :: ac_r_lim, ac_s_lim, aq_lim
        INTEGER :: ib, nnb
        REAL,    DIMENSION(1:nni+1)  :: kb2  ! [1/cm^2]
        REAL,    DIMENSION(1:nni+1)  :: ab   ! [dimensionless]
        REAL,    DIMENSION(1:nni+1)  :: ab2  ! [dimensionless]
        REAL,    DIMENSION(1:nni+1)  :: mpb  ! [keV]
        REAL,    DIMENSION(1:nni+1)  :: mbpb ! [dimensionless]
        REAL    :: vp                        ! [cm/s]
        REAL    :: vp2                       ! [cm^2/s^2]
        REAL    :: kd2, k2                   ! [1/cm^2]
        REAL    :: kd, k                     ! [1/cm]
        REAL    :: a, zp2                    ! [dimensionless]
        REAL    :: c1                        ! [keV/cm]
        REAL    :: c2                        ! [dimensionless]
        REAL    :: ar1, ar2                  ! [dimensionless]
        REAL    :: etbar, etbar2             ! [dimensionless]

        nnb =nni+1
        vp  = CC*SQRT(2*ep/mp)      ! [cm/s]
        vp2 = vp*vp                 ! [cm^2/s^2]
        kb2 = DEBYE2*zb*zb*nb*betab ! [1/cm^2]
        kd2 = SUM(kb2)              ! [1/cm^2]
        kd  = SQRT(kd2)             ! [1/cm]
        k2  = kb2(1)                ! [1/cm^2]  k2=k_e^2
        k   = SQRT(k2)              ! [1/cm]    k =k_e
        zp2 = zp**2                 ! [dimensionless]
                                    ! ab=(1/2) betab(ib)*mbc2(ib)*vp2/CC2
        ab  =0.5*betab*mb*vp2/CC2   ! [dimensionless]
        mpb = mp*mb/(mp+mb)         ! [keV]
        mbpb= mb/mpb                ! [dimensionless]
!
! initialize A-coefficients
!
        a_tot_lim = 0  ! electron + ion
        a_i_lim   = 0  ! ion contribution
        a_e_lim   = 0  ! electron contribution
        ac_tot_lim= 0  ! classical total
        ac_e_lim  = 0  ! classical electron
        ac_i_lim  = 0  ! classical ion
        aq_tot_lim= 0  ! quantum total
        aq_e_lim  = 0  ! quantum electron
        aq_i_lim  = 0  ! quantum ion
!
        DO ib=1,nni+1
        IF (zb(ib) .NE. 0.) THEN

           a=ab(ib)                    ! [dimensionless]
           c1=2*zp2*BEKEV*kb2(ib)*A0CM ! [keV/cm]
           c1=c1*1.E-7                 ! [MeV/micron]
           c2=SQRT(a/PI)               ! [dimensionless]
```

```
!
! singular: asymptotic low energy form
!
          ac_s_lim=-(2./3. - 0.4*a)*(LOG(betab(ib)*BEKEV*ABS(zp*zb(ib))* &
          0.5*k*AOCM*mbpb(ib) ) + 2*GAMMA) - (4./15.)*a
          ac_s_lim=c1*c2*ac_s_lim
!
! regular: asymptotic low energy form
!
          ab2 = SQRT(ab)               ! [dimensionless]
          ar1 =-2*SUM(kb2*ab)/k2/5.    ! [dimensionless] coeff for A_reg with E<<T
          ar2 = SUM(kb2*ab2)/k2        ! [dimensionless] coeff for A_reg with E<<T
          ar2 = ar2*ar2*PI/30.         !
          ac_r_lim=-c1*c2*((THIRD - 0.2*a)*(LOG(kd2/k2)+1) + ar1 + ar2 )
!
! quantum: asymptotic low energy form: etbar defined with thermal velocity
! [$\bar eta_{pb} = e_p e_b/4\pi \hbar \bar v_b $  with $\bar v_b^2 = 3 T_b/m_b$]
!
          etbar=4.2115E-3*ABS(zp*zb(ib))*SQRT(betab(ib)*mb(ib))
          etbar2=etbar*etbar
          IF (ib==1) THEN
             aq_lim=LOG(1.5*etbar2)/3 + GAMMA  ! electrons only eta_pe << 1
             aq_lim=c1*c2*aq_lim
          ELSE
             aq_lim=-1./(27*etbar2)
             aq_lim=c1*c2*aq_lim
          ENDIF
          CALL a_collect(ib,nnb,ac_s_lim,ac_r_lim,aq_lim,a_tot_lim,a_e_lim, &
            a_i_lim,ac_tot_lim,ac_e_lim,ac_i_lim,aq_tot_lim,aq_e_lim,aq_i_lim)
        ENDIF
        ENDDO
      END SUBROUTINE coeff_bps_small_E
```

3. High Energy Asymptotics

acoeff.f90 cont.:

```
!
! ROUTINE: SUBROUTINE coeff_bps_high_EE(nni, ep, zp, mp, betab, zb, mb, nb, &
!   a_tot_lim, a_i_lim, a_e_lim, ac_tot_lim, ac_i_lim, ac_e_lim, aq_tot_lim,&
!   aq_i_lim, aq_e_lim)
!
! Returns high energy asymptotic regimes. For the ions this means E_p >> T.
! For electrons there are two regimes:
! (i)  extreme high energy E_p >> (m_I/m_e)*T,
! (ii) intermediate high energy T << E_p << (m_I/m_e)*T.
! Currently the two electron regimes must be swapped in/out by hand.
!
! UNITS: A_b has units of [MeV/micron] (subject to change in updates)
!
! The incident projectile and the background plasma.
!
! projectile input quantities:
! ep : classical kinetic energy of the projectile [keV]
! zp : charge of the projectile in units of Z_p [dimensionless]
! mp : mass of the projectile [keV], i.e. mp = mp[grams]*c^2
!
! plasma input quantities:
! nni  : Number of total plasma species = number ion species + 1
! zb   : Charges of the plasma species. By convention zp(1) is the
```

```
!      : electron plasma component. [dimensionless, Array]
! betab: Inverse temperatures of the plasma components. For an
!        electron-ion plasma, set betab(1)=1/T_e and all other
!        values of the array to 1/T_I.
! mb   : Masses of the plasma species [keV].
! nb   : Number densities of the plasma species [cm^-3].
!
! OUTPUT: a_tot_lim, a_i_lim, a_e_lim, ac_tot_lim, ac_i+lim, ac_e_lim,
!         aq_tot_lim, aq_i_lim, aq_e_lim
!
! classical electron  : ac_e_lim
! classical ion       : ac_i_lim [sum over all ions]
! classical total     : ac_tot_lim = ac_e_lim + ac_i_lim
! quantum   electron  : aq_e_lim
! quantum   ion       : aq_i_lim [sum over all ions]
! quantum   total     : a_tot_lim = aq_e_lim + aq_i_lim
! total     electric  : a_e_lim = ac_e_lim + aq_e_lim
! total     ion       : a_i_lim = ac_i_lim + aq_i_lim
! total               ! a_tot_lim = a_e_lim + a_i_lim
!
      SUBROUTINE coeff_bps_high_E(nni, ep, zp, mp, betab, zb, mb, nb,   &
            a_tot_lim, a_i_lim, a_e_lim, ac_tot_lim, ac_i_lim, ac_e_lim, &
            aq_tot_lim, aq_i_lim, aq_e_lim)
      USE physvars
      USE mathvars
        IMPLICIT NONE
        INTEGER,                          INTENT(IN)  :: nni    !  number of ions
        REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: betab  !  temp array    [1/keV]
        REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: mb     !  mass array    [keV]
        REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: nb     !  density array [1/cc]
        REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: zb     !  charge array
                                                           !
                                                           ! Projectile
        REAL,                          INTENT(IN)  :: ep     !  projectile energy [keV]
        REAL,                          INTENT(IN)  :: mp     !  projectile mass   [keV]
        REAL,                          INTENT(IN)  :: zp     !  projectile charge
                                                           !
                                                             ! A-coeffs [MeV/micron]
        REAL,                          INTENT(OUT) :: a_tot_lim  !  electron + ion
        REAL,                          INTENT(OUT) :: a_i_lim    !  ion contribution
        REAL,                          INTENT(OUT) :: a_e_lim    !  electron contributi
        REAL,                          INTENT(OUT) :: ac_tot_lim !  classical
        REAL,                          INTENT(OUT) :: ac_i_lim   !  classical
        REAL,                          INTENT(OUT) :: ac_e_lim   !  classical
        REAL,                          INTENT(OUT) :: aq_tot_lim !  quantum
        REAL,                          INTENT(OUT) :: aq_i_lim   !  quantum
        REAL,                          INTENT(OUT) :: aq_e_lim   !  quantum

        REAL    :: ac_r_lim, ac_s_lim, aq_lim
        INTEGER :: ib, nnb
        REAL    :: vp                          ! [cm/s]
        REAL    :: vp2                         ! [cm^2/s^2]
        REAL    :: a, zp2                      ! [dimensionless]
        REAL    :: c1, cs                      ! [keV/cm]
        REAL    :: c2                          ! [dimensionless]
        REAL    :: k                           ! [1/cm]
        REAL    :: k2, ke2                     ! [1/cm^2]
        REAL    :: eta                         ! [dimensionless]
        REAL    :: te, mec2, mpec22            ! [keV]
        REAL,    DIMENSION(1:nni+1)  :: ab   ! [dimensionless]
        REAL,    DIMENSION(1:nni+1)  :: mpb  ! [keV]
        REAL,    DIMENSION(1:nni+1)  :: kb2  ! [1/cm^2
!
! omi2, and omi needed only for
```

```
! E >> (mI/me)*T: extreme high energy limit for electrons
!
!       REAL    :: omi2, omi                 ! [1/s^2, 1/s]]

        nnb = nni+1
        vp  = CC*SQRT(2*ep/mp)      ! [cm/s]
        vp2 = vp*vp                 ! [cm^2/s^2]
        kb2 = DEBYE2*zb*zb*nb*betab ! [1/cm^2]
        k2  = kb2(1)                ! [1/cm^2]  k2=k_e^2
        k   = SQRT(k2)              ! [1/cm]    k =k_e
        zp2 = zp**2                 ! [dimensionless]
                                    ! ab=(1/2) betab(ib)*mb(ib)*vp2/CC2
        ab  =0.5*betab*mb*vp2/CC2   ! [dimensionless]
        mpb = mp*mb/(mp+mb)         ! [keV]
!
! initialize A-coefficients
!
        a_tot_lim = 0  ! electron + ion
        a_i_lim   = 0  ! ion contribution
        a_e_lim   = 0  ! electron contribution
        ac_tot_lim= 0  ! classical total
        ac_e_lim  = 0  ! classical electron
        ac_i_lim  = 0  ! classical ion
        aq_tot_lim= 0  ! quantum total
        aq_e_lim  = 0  ! quantum electron
        aq_i_lim  = 0  ! quantum ion
!
        DO ib=1,nni+1
        IF (zb(ib) .NE. 0.) THEN

           a=ab(ib)                     ! [dimensionless]
           c1=2*zp2*BEKEV*kb2(ib)*AOCM ! [keV/cm]
           c1=c1*1.E-7                  ! [MeV/micron]
           c2=SQRT(a/PI)                ! [dimensionless]
!
! singular: asymptotic high energy form [need electrons]
!
! At this point I only have an asymptotic form for the total
! electron contribution (classical + quantum = sing + reg + quantum).
! I'll write this expression to ac_s_lim for now. This will give
! aq_lim=0 and ac_lim=a_e.  FIX LATER.
!
           IF (ib == 1) THEN
!
! T << E << (mI/me)*T: intermediate high energy limit for electrons
!
              te=1./betab(ib)
              mpec22=mpb(ib)**2
              mec2  =mb(ib)
              ke2   =kb2(ib)
              ac_s_lim=THIRD*(LOG(8*te*mpec22/(mec2*HBARC**2*ke2)) - GAMMA -1)
              ac_s_lim=c1*c2*ac_s_lim              ! [MeV/micron]
!
! E >> (mI/me)*T: extreme high energy limit for electrons
!
!!              omi2=OMEGI2*zb(ib)*zb(ib)*nb(ib)*AMUKEV/mb(ib) ! [1/s^2]
!!              omi =SQRT(omi2)
!!              ac_s_lim=0.5*c1*LOG(2*mpb(ib)*vp2/(HBARC*CC*omi))/ab(ib)
           ELSE
              cs=0.5*c1/ab(ib)
              ac_s_lim=(LOG(ABS(zp*zb(ib))*BEKEV*& ! [dimensionless]
                k*AOCM*CC2/(mpb(ib)*vp2)) + GAMMA) !
              ac_s_lim=-cs*ac_s_lim                ! [MeV/micron]
           ENDIF
!
! regular: asymptotic high energy form [need electrons]
```

```
!
           IF (ib == 1) THEN
              ac_r_lim=0
           ELSE
               ac_r_lim=-0.25*c1/ab(ib)                          ! [MeV/micron]
           ENDIF
!
! quantum: asymptotic high energy form [need electrons]
!
           IF (ib == 1) THEN
              aq_lim=0
           ELSE
              eta =ABS(zp*zb(ib))*2.1870E8/vp  ! [dimensionless] quantum parameter
              aq_lim=LOG(eta) + GAMMA
              aq_lim=aq_lim*c1/a/2
           ENDIF
           CALL a_collect(ib,nnb,ac_s_lim,ac_r_lim,aq_lim,a_tot_lim,a_e_lim, &
             a_i_lim,ac_tot_lim,ac_e_lim,ac_i_lim,aq_tot_lim,aq_e_lim,aq_i_lim)
         ENDIF
         ENDDO
      END SUBROUTINE coeff_bps_high_E
```

4. Small Energy Asymptotics

acoeff.f90:

```
      SUBROUTINE coeff_bps_small_E(nni, ep, zp, mp, betab, zb, mb, nb,   &
            a_tot_lim, a_i_lim, a_e_lim, ac_tot_lim, ac_i_lim, ac_e_lim, &
            aq_tot_lim, aq_i_lim, aq_e_lim)
      USE physvars
      USE mathvars
        IMPLICIT NONE
        INTEGER,                          INTENT(IN)  :: nni    !  number of ions
        REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: betab  !  temp array    [1/keV]
        REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: mb     !  mass array    [keV]
        REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: nb     !  density array [1/cc]
        REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: zb     !  charge array
                                                           !
                                                           ! Projectile
        REAL,                          INTENT(IN)  :: ep     !  projectile energy [keV]
        REAL,                          INTENT(IN)  :: mp     !  projectile mass   [keV]
        REAL,                          INTENT(IN)  :: zp     !  projectile charge
                                                           !
                                                             ! A-coeffs [MeV/micron
        REAL,                          INTENT(OUT) :: a_tot_lim  !  electron + ion
        REAL,                          INTENT(OUT) :: a_i_lim    !  ion contribution
        REAL,                          INTENT(OUT) :: a_e_lim    !  electron contributi
        REAL,                          INTENT(OUT) :: ac_tot_lim !  classical
        REAL,                          INTENT(OUT) :: ac_i_lim   !  classical
        REAL,                          INTENT(OUT) :: ac_e_lim   !  classical
        REAL,                          INTENT(OUT) :: aq_tot_lim !  quantum
        REAL,                          INTENT(OUT) :: aq_i_lim   !  quantum
        REAL,                          INTENT(OUT) :: aq_e_lim   !  quantum

        REAL    :: ac_r_lim, ac_s_lim, aq_lim
        INTEGER :: ib, nnb
        REAL,    DIMENSION(1:nni+1)  :: kb2  ! [1/cm^2]
        REAL,    DIMENSION(1:nni+1)  :: ab   ! [dimensionless]
        REAL,    DIMENSION(1:nni+1)  :: ab2  ! [dimensionless]
```

```
        REAL,    DIMENSION(1:nni+1)  :: mpb  ! [keV]
        REAL,    DIMENSION(1:nni+1)  :: mbpb ! [dimensionless]
        REAL    :: vp                        ! [cm/s]
        REAL    :: vp2                       ! [cm^2/s^2]
        REAL    :: kd2, k2                   ! [1/cm^2]
        REAL    :: kd, k                     ! [1/cm]
        REAL    :: a, zp2                    ! [dimensionless]
        REAL    :: c1                        ! [keV/cm]
        REAL    :: c2                        ! [dimensionless]
        REAL    :: ar1, ar2                  ! [dimensionless]
        REAL    :: etbar, etbar2             ! [dimensionless]

        nnb =nni+1
        vp  = CC*SQRT(2*ep/mp)      ! [cm/s]
        vp2 = vp*vp                 ! [cm^2/s^2]
        kb2 = DEBYE2*zb*zb*nb*betab ! [1/cm^2]
        kd2 = SUM(kb2)              ! [1/cm^2]
        kd  = SQRT(kd2)             ! [1/cm]
        k2  = kb2(1)                ! [1/cm^2]  k2=k_e^2
        k   = SQRT(k2)              ! [1/cm]    k =k_e
        zp2 = zp**2                 ! [dimensionless]
                                    ! ab=(1/2) betab(ib)*mbc2(ib)*vp2/CC2
        ab  =0.5*betab*mb*vp2/CC2   ! [dimensionless]
        mpb = mp*mb/(mp+mb)         ! [keV]
        mbpb= mb/mpb                ! [dimensionless]
!
! initialize A-coefficients
!
        a_tot_lim = 0  ! electron + ion
        a_i_lim   = 0  ! ion contribution
        a_e_lim   = 0  ! electron contribution
        ac_tot_lim= 0  ! classical total
        ac_e_lim  = 0  ! classical electron
        ac_i_lim  = 0  ! classical ion
        aq_tot_lim= 0  ! quantum total
        aq_e_lim  = 0  ! quantum electron
        aq_i_lim  = 0  ! quantum ion
!
        DO ib=1,nni+1
        IF (zb(ib) .NE. 0.) THEN

           a=ab(ib)                     ! [dimensionless]
           c1=2*zp2*BEKEV*kb2(ib)*A0CM ! [keV/cm]
           c1=c1*1.E-7                  ! [MeV/micron]
           c2=SQRT(a/PI)                ! [dimensionless]
!
! singular: asymptotic low energy form
!
           ac_s_lim=-(2./3. - 0.4*a)*(LOG(betab(ib)*BEKEV*ABS(zp*zb(ib))* &
           0.5*k*A0CM*mbpb(ib) ) + 2*GAMMA) - (4./15.)*a
           ac_s_lim=c1*c2*ac_s_lim
!
! regular: asymptotic low energy form
!
           ab2 = SQRT(ab)               ! [dimensionless]
           ar1 =-2*SUM(kb2*ab)/k2/5.    ! [dimensionless] coeff for A_reg with E<<T
           ar2 = SUM(kb2*ab2)/k2        ! [dimensionless] coeff for A_reg with E<<T
           ar2 = ar2*ar2*PI/30.         !
           ac_r_lim=-c1*c2*((THIRD - 0.2*a)*(LOG(kd2/k2)+1) + ar1 + ar2 )
!
! quantum: asymptotic low energy form: etbar defined with thermal velocity
! [$\bar eta_{pb} = e_p e_b/4\pi \hbar \bar v_b $  with $\bar v_b^2 = 3 T_b/m_b$]
!
           etbar=4.2115E-3*ABS(zp*zb(ib))*SQRT(betab(ib)*mb(ib))
           etbar2=etbar*etbar
```

```
          IF (ib==1) THEN
             aq_lim=LOG(1.5*etbar2)/3 + GAMMA  ! electrons only eta_pe << 1
             aq_lim=c1*c2*aq_lim
          ELSE
             aq_lim=-1./(27*etbar2)
             aq_lim=c1*c2*aq_lim
          ENDIF
          CALL a_collect(ib,nnb,ac_s_lim,ac_r_lim,aq_lim,a_tot_lim,a_e_lim, &
            a_i_lim,ac_tot_lim,ac_e_lim,ac_i_lim,aq_tot_lim,aq_e_lim,aq_i_lim)
        ENDIF
        ENDDO
      END SUBROUTINE coeff_bps_small_E
```

5. High Energy Asymptotics

Medium-high energy electrons:

acoeff.f90:

```
!
! ROUTINE: SUBROUTINE coeff_bps_high_E(nni, ep, zp, mp, betab, zb, mb, nb, &
!   a_tot_lim, a_i_lim, a_e_lim, ac_tot_lim, ac_i_lim, ac_e_lim, aq_tot_lim,&
!   aq_i_lim, aq_e_lim)
!
! Returns high energy asymptotic regimes. For the ions this means E_p >> T.
! For electrons there are two regimes:
! (i)  extreme high energy E_p >> (m_I/m_e)*T [coeff_bps_very_high_E]
! (ii) intermediate high energy T << E_p << (m_I/m_e)*T [this routine]
!
! UNITS: A_b has units of [MeV/micron] (subject to change in updates)
!
! The incident projectile and the background plasma.
!
! projectile input quantities:
! ep : classical kinetic energy of the projectile [keV]
! zp : charge of the projectile in units of Z_p [dimensionless]
! mp : mass of the projectile [keV], i.e. mp = mp[grams]*c^2
!
! plasma input quantities:
! nni  : Number of total plasma species = number ion species + 1
! zb   : Charges of the plasma species. By convention zp(1) is the
!      : electron plasma component. [dimensionless, Array]
! betab: Inverse temperatures of the plasma components. For an
!        electron-ion plasma, set betab(1)=1/T_e and all other
!        values of the array to 1/T_I.
! mb   : Masses of the plasma species [keV].
! nb   : Number densities of the plasma species [cm^-3].
!
! OUTPUT: a_tot_lim, a_i_lim, a_e_lim, ac_tot_lim, ac_i+lim, ac_e_lim,
!         aq_tot_lim, aq_i_lim, aq_e_lim
!
! classical electron  : ac_e_lim
! classical ion       : ac_i_lim [sum over all ions]
! classical total     : ac_tot_lim = ac_e_lim + ac_i_lim
! quantum   electron  : aq_e_lim
! quantum   ion       : aq_i_lim [sum over all ions]
! quantum   total     : a_tot_lim = aq_e_lim + aq_i_lim
! total     electric  : a_e_lim = ac_e_lim + aq_e_lim
! total     ion       : a_i_lim = ac_i_lim + aq_i_lim
! total               ! a_tot_lim = a_e_lim + a_i_lim
!
```

```
      SUBROUTINE coeff_bps_high_E(nni, ep, zp, mp, betab, zb, mb, nb,    &
            a_tot_lim, a_i_lim, a_e_lim, ac_tot_lim, ac_i_lim, ac_e_lim, &
            aq_tot_lim, aq_i_lim, aq_e_lim)
      USE physvars
      USE mathvars
        IMPLICIT NONE
        INTEGER,                          INTENT(IN)  :: nni    !  number of ions
        REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: betab  !  temp array    [1/keV]
        REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: mb     !  mass array    [keV]
        REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: nb     !  density array [1/cc]
        REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: zb     !  charge array
                                                           !
                                                           ! Projectile
        REAL,                          INTENT(IN)  :: ep     !  projectile energy [keV]
        REAL,                          INTENT(IN)  :: mp     !  projectile mass   [keV]
        REAL,                          INTENT(IN)  :: zp     !  projectile charge
                                                           !
                                                              ! A-coeffs [MeV/micron]
        REAL,                          INTENT(OUT) :: a_tot_lim  !  electron + ion
        REAL,                          INTENT(OUT) :: a_i_lim    !  ion contribution
        REAL,                          INTENT(OUT) :: a_e_lim    !  electron contributi
        REAL,                          INTENT(OUT) :: ac_tot_lim !  classical
        REAL,                          INTENT(OUT) :: ac_i_lim   !  classical
        REAL,                          INTENT(OUT) :: ac_e_lim   !  classical
        REAL,                          INTENT(OUT) :: aq_tot_lim !  quantum
        REAL,                          INTENT(OUT) :: aq_i_lim   !  quantum
        REAL,                          INTENT(OUT) :: aq_e_lim   !  quantum

        REAL    :: ac_r_lim, ac_s_lim, aq_lim
        INTEGER :: ib, nnb
        REAL    :: vp                          ! [cm/s]
        REAL    :: vp2                         ! [cm^2/s^2]
        REAL    :: a, zp2                      ! [dimensionless]
        REAL    :: c1, cs                      ! [keV/cm]
        REAL    :: c2                          ! [dimensionless]
        REAL    :: k                           ! [1/cm]
        REAL    :: k2, ke2                     ! [1/cm^2]
        REAL    :: eta                         ! [dimensionless]
        REAL    :: te, mec2, mpec22            ! [keV]
        REAL,    DIMENSION(1:nni+1)  :: ab   ! [dimensionless]
        REAL,    DIMENSION(1:nni+1)  :: mpb  ! [keV]
        REAL,    DIMENSION(1:nni+1)  :: kb2  ! [1/cm^2
!
! omi2, and omi needed only for
! E >> (mI/me)*T: extreme high energy limit for electrons
!
!       REAL    :: omi2, omi                   ! [1/s^2, 1/s]]

        nnb = nni+1
        vp  = CC*SQRT(2*ep/mp)       ! [cm/s]
        vp2 = vp*vp                  ! [cm^2/s^2]
        kb2 = DEBYE2*zb*zb*nb*betab  ! [1/cm^2]
        k2  = kb2(1)                 ! [1/cm^2]  k2=k_e^2
        k   = SQRT(k2)               ! [1/cm]    k =k_e
        zp2 = zp**2                  ! [dimensionless]
                                     ! ab=(1/2) betab(ib)*mb(ib)*vp2/CC2
        ab  =0.5*betab*mb*vp2/CC2    ! [dimensionless]
        mpb = mp*mb/(mp+mb)          ! [keV]
!
! initialize A-coefficients
!
        a_tot_lim = 0  ! electron + ion
        a_i_lim   = 0  ! ion contribution
        a_e_lim   = 0  ! electron contribution
```

```
        ac_tot_lim= 0  ! classical total
        ac_e_lim  = 0  ! classical electron
        ac_i_lim  = 0  ! classical ion
        aq_tot_lim= 0  ! quantum total
        aq_e_lim  = 0  ! quantum electron
        aq_i_lim  = 0  ! quantum ion
!
        DO ib=1,nni+1
        IF (zb(ib) .NE. 0.) THEN

           a=ab(ib)                      ! [dimensionless]
           c1=2*zp2*BEKEV*kb2(ib)*A0CM ! [keV/cm]
           c1=c1*1.E-7                   ! [MeV/micron]
           c2=SQRT(a/PI)                 ! [dimensionless]
!
! singular: asymptotic high energy form [need electrons]
!
! At this point I only have an asymptotic form for the total
! electron contribution (classical + quantum = sing + reg + quantum).
! I'll write this expression to ac_s_lim for now. This will give
! aq_lim=0 and ac_lim=a_e.  FIX LATER.
!
           IF (ib == 1) THEN
!
! T << E << (mI/me)*T: intermediate high energy limit for electrons
!
              te=1./betab(ib)
              mpec22=mpb(ib)**2
              mec2  =mb(ib)
              ke2   =kb2(ib)
              ac_s_lim=THIRD*(LOG(8*te*mpec22/(mec2*HBARC**2*ke2)) - GAMMA -1)
              ac_s_lim=c1*c2*ac_s_lim              ! [MeV/micron]
           ELSE
              cs=0.5*c1/ab(ib)
              ac_s_lim=(LOG(ABS(zp*zb(ib))*BEKEV*& ! [dimensionless]
                k*A0CM*CC2/(mpb(ib)*vp2)) + GAMMA) !
              ac_s_lim=-cs*ac_s_lim                ! [MeV/micron]
           ENDIF
!
! regular: asymptotic high energy form [need electrons]
!
           IF (ib == 1) THEN
              ac_r_lim=0
           ELSE
               ac_r_lim=-0.25*c1/ab(ib)                        ! [MeV/micron]
           ENDIF
!
! quantum: asymptotic high energy form [need electrons]
!
           IF (ib == 1) THEN
              aq_lim=0
           ELSE
              eta =ABS(zp*zb(ib))*2.1870E8/vp  ! [dimensionless] quantum parameter
              aq_lim=LOG(eta) + GAMMA
              aq_lim=aq_lim*c1/a/2
           ENDIF
           CALL a_collect(ib,nnb,ac_s_lim,ac_r_lim,aq_lim,a_tot_lim,a_e_lim, &
             a_i_lim,ac_tot_lim,ac_e_lim,ac_i_lim,aq_tot_lim,aq_e_lim,aq_i_lim)
        ENDIF
        ENDDO
      END SUBROUTINE coeff_bps_high_E
```

Extreme-high energy electrons:

acoeff.f90:

```
      SUBROUTINE coeff_bps_very_high_E(nni, ep, zp, mp, betab, zb, mb, nb, &
            a_tot_lim, a_i_lim, a_e_lim, ac_tot_lim, ac_i_lim, ac_e_lim,   &
            aq_tot_lim, aq_i_lim, aq_e_lim)
      USE physvars
      USE mathvars
        IMPLICIT NONE
        INTEGER,                        INTENT(IN)  :: nni    !  number of ions
        REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: betab  !  temp array    [1/keV]
        REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: mb     !  mass array    [keV]
        REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: nb     !  density array [1/cc]
        REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: zb     !  charge array
                                                           !
                                                           ! Projectile
        REAL,                        INTENT(IN)  :: ep     !  projectile energy [keV]
        REAL,                        INTENT(IN)  :: mp     !  projectile mass   [keV]
        REAL,                        INTENT(IN)  :: zp     !  projectile charge
                                                           !
                                                             ! A-coeffs [MeV/micron
        REAL,                        INTENT(OUT) :: a_tot_lim  !  electron + ion
        REAL,                        INTENT(OUT) :: a_i_lim    !  ion contribution
        REAL,                        INTENT(OUT) :: a_e_lim    !  electron contributi
        REAL,                        INTENT(OUT) :: ac_tot_lim !  classical
        REAL,                        INTENT(OUT) :: ac_i_lim   !  classical
        REAL,                        INTENT(OUT) :: ac_e_lim   !  classical
        REAL,                        INTENT(OUT) :: aq_tot_lim !  quantum
        REAL,                        INTENT(OUT) :: aq_i_lim   !  quantum
        REAL,                        INTENT(OUT) :: aq_e_lim   !  quantum

        REAL    :: omi2, omi
        REAL    :: ac_r_lim, ac_s_lim, aq_lim
        INTEGER :: ib, nnb
        REAL    :: vp                          ! [cm/s]
        REAL    :: vp2                         ! [cm^2/s^2]
        REAL    :: a, zp2                      ! [dimensionless]
        REAL    :: c1, cs                      ! [keV/cm]
        REAL    :: c2                          ! [dimensionless]
        REAL    :: k                           ! [1/cm]
        REAL    :: k2                          ! [1/cm^2]
        REAL    :: eta                         ! [dimensionless]
        REAL,    DIMENSION(1:nni+1)  :: ab     ! [dimensionless]
        REAL,    DIMENSION(1:nni+1)  :: mpb    ! [keV]
        REAL,    DIMENSION(1:nni+1)  :: kb2    ! [1/cm^2
!
! omi2, and omi needed only for
! E >> (mI/me)*T: extreme high energy limit for electrons
!
!       REAL    :: omi2, omi                   ! [1/s^2, 1/s]]

        nnb = nni+1
        vp  = CC*SQRT(2*ep/mp)       ! [cm/s]
        vp2 = vp*vp                  ! [cm^2/s^2]
        kb2 = DEBYE2*zb*zb*nb*betab  ! [1/cm^2]
        k2  = kb2(1)                 ! [1/cm^2]  k2=k_e^2
        k   = SQRT(k2)               ! [1/cm]    k =k_e
        zp2 = zp**2                  ! [dimensionless]
                                     ! ab=(1/2) betab(ib)*mb(ib)*vp2/CC2
        ab  =0.5*betab*mb*vp2/CC2    ! [dimensionless]
        mpb = mp*mb/(mp+mb)          ! [keV]
!
! initialize A-coefficients
!
        a_tot_lim = 0  ! electron + ion
        a_i_lim   = 0  ! ion contribution
```

```
        a_e_lim   = 0  ! electron contribution
        ac_tot_lim= 0  ! classical total
        ac_e_lim  = 0  ! classical electron
        ac_i_lim  = 0  ! classical ion
        aq_tot_lim= 0  ! quantum total
        aq_e_lim  = 0  ! quantum electron
        aq_i_lim  = 0  ! quantum ion
!
        DO ib=1,nni+1
        IF (zb(ib) .NE. 0.) THEN

           a=ab(ib)                     ! [dimensionless]
           c1=2*zp2*BEKEV*kb2(ib)*A0CM ! [keV/cm]
           c1=c1*1.E-7                  ! [MeV/micron]
           c2=SQRT(a/PI)                ! [dimensionless]
!
! singular: asymptotic high energy form [need electrons]
!
! At this point I only have an asymptotic form for the total
! electron contribution (classical + quantum = sing + reg + quantum).
! I'll write this expression to ac_s_lim for now. This will give
! aq_lim=0 and ac_lim=a_e.  FIX LATER.
!
           IF (ib == 1) THEN
!
! E >> (mI/me)*T: extreme high energy limit for electrons
!
              omi2=OMEGI2*zb(ib)*zb(ib)*nb(ib)*AMUKEV/mb(ib) ! [1/s^2]
              omi =SQRT(omi2)
              ac_s_lim=0.5*c1*LOG(2*mpb(ib)*vp2/(HBARC*CC*omi))/ab(ib)
           ELSE
              cs=0.5*c1/ab(ib)
              ac_s_lim=(LOG(ABS(zp*zb(ib))*BEKEV*& ! [dimensionless]
                k*A0CM*CC2/(mpb(ib)*vp2)) + GAMMA) !
              ac_s_lim=-cs*ac_s_lim               ! [MeV/micron]
           ENDIF
!
! regular: asymptotic high energy form [need electrons]
!
           IF (ib == 1) THEN
              ac_r_lim=0
           ELSE
               ac_r_lim=-0.25*c1/ab(ib)                      ! [MeV/micron]
           ENDIF
!
! quantum: asymptotic high energy form [need electrons]
!
           IF (ib == 1) THEN
              aq_lim=0
           ELSE
              eta =ABS(zp*zb(ib))*2.1870E8/vp  ! [dimensionless] quantum parameter
              aq_lim=LOG(eta) + GAMMA
              aq_lim=aq_lim*c1/a/2
           ENDIF
           CALL a_collect(ib,nnb,ac_s_lim,ac_r_lim,aq_lim,a_tot_lim,a_e_lim, &
             a_i_lim,ac_tot_lim,ac_e_lim,ac_i_lim,aq_tot_lim,aq_e_lim,aq_i_lim)
        ENDIF
        ENDDO
      END SUBROUTINE coeff_bps_very_high_E
```