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A-Coefficient Study

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A-Coefficient Study

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Abstract

This is a study of the asymptotic behavior of the \mathcal{A} -coefficients from `Clog/acoef.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.

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I. A-COEFFICIENTS AS A FUNCTION OF ENERGY

The A-coefficients take the form

$$\mathcal{A}_b = \mathcal{A}_b^c + \mathcal{A}_b^{\Delta Q} \quad \text{where} \quad \mathcal{A}_b^c = \mathcal{A}_{b,s}^c + \mathcal{A}_{b,r}^c, \quad (1.1)$$

with

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

$$\mathcal{A}_{b,r}^c = \frac{e_p^2}{4\pi} \frac{i}{2\pi} \int_{-1}^1 d \cos \theta \cos \theta \frac{\rho_b(v_p \cos \theta)}{\rho_{\text{total}}(v_p \cos \theta)} F(v_p \cos \theta) \ln \left\{ \frac{F(v_p \cos \theta)}{K^2} \right\}, \quad (1.3)$$

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

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

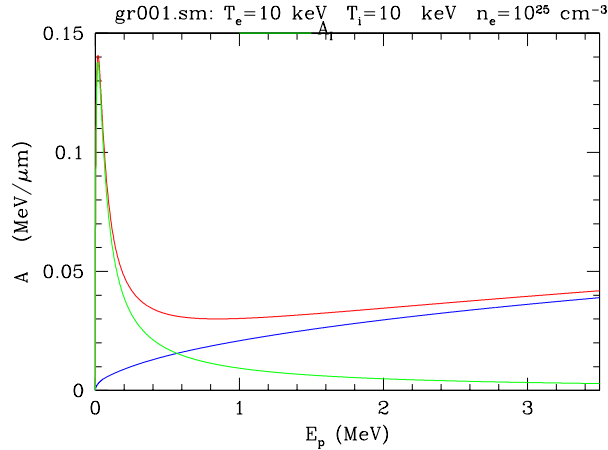


FIG. 1: Electron and ion components: $n_e = 10^{25} \text{ cm}^{-3}$, $T_e = 10 \text{ keV}$, $T_i = 10 \text{ keV}$. [gr001.f90, gr001.sm, gr001.dat, gr001.eps]

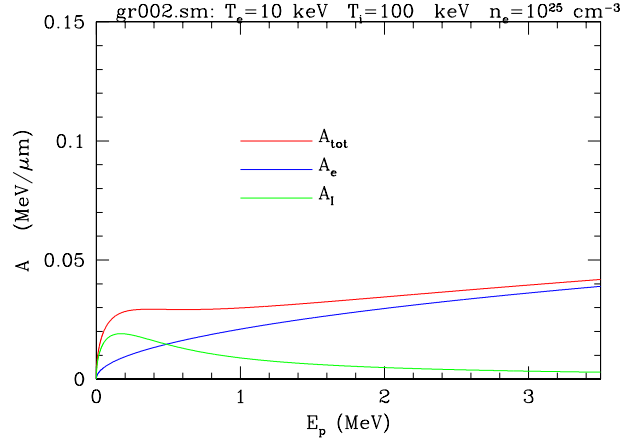


FIG. 2: Electron and ion components: $n_e = 10^{25} \text{ cm}^{-3}$, $T_e = 10 \text{ keV}$, $T_i = 100 \text{ keV}$. [gr002.f90, gr002.sm, gr002.dat, gr002.eps]

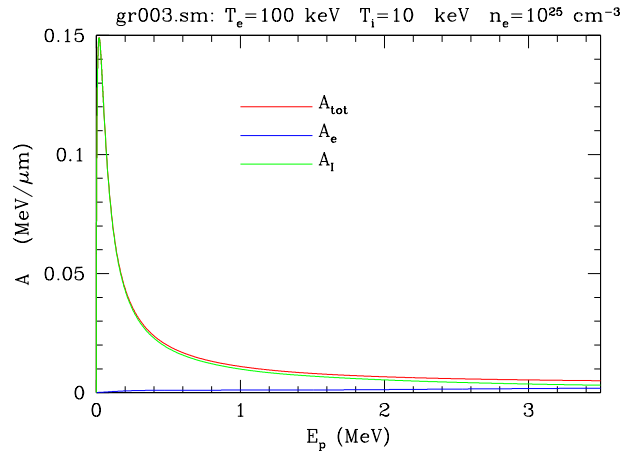


FIG. 3: Electron and ion components: $n_e = 10^{25} \text{ cm}^{-3}$, $T_e = 100 \text{ keV}$, $T_i = 10 \text{ keV}$. [gr003.f90, gr003.sm, gr003.dat, gr003.eps]

II. SMALL ENERGY ASYMPTOTIC BEHAVIOR

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

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

with

$$A_b^C = \frac{2}{3} \left[\ln \left(\frac{16\pi}{e_p e_b \beta_b \kappa_D} \frac{m_{pb}}{m_b} \right) - \frac{1}{2} - 2\gamma \right] \quad (2.2)$$

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

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:

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

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

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

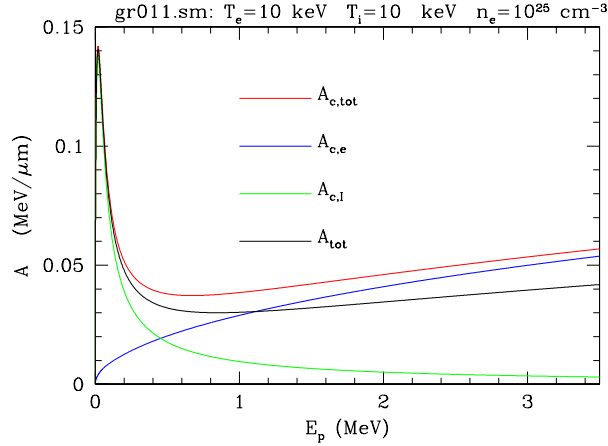


FIG. 4: The classical contributions to the A-coefficient, with the total (classical + quantum) in black. [gr001.f90, gr011.sm, gr001.dat, gr011.eps]

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 $T_e = 10 \text{ keV}$ and $T_i = 10 \text{ keV}$

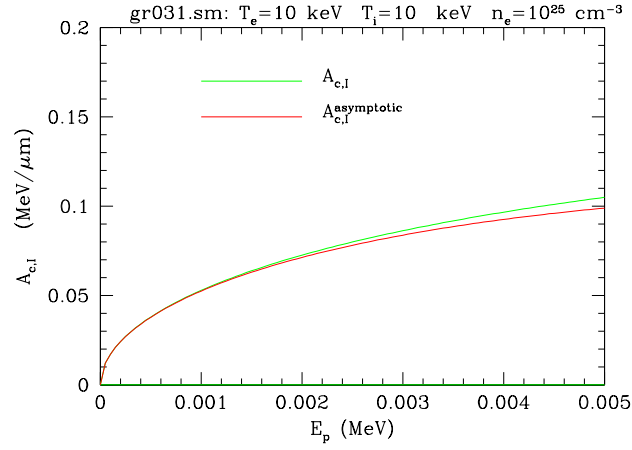


FIG. 5: Asymptotic classical ion contribution at low energies. [gr001.f90, gr031.sm, gr001.dat, gr001.smallE.dat, gr031.eps]

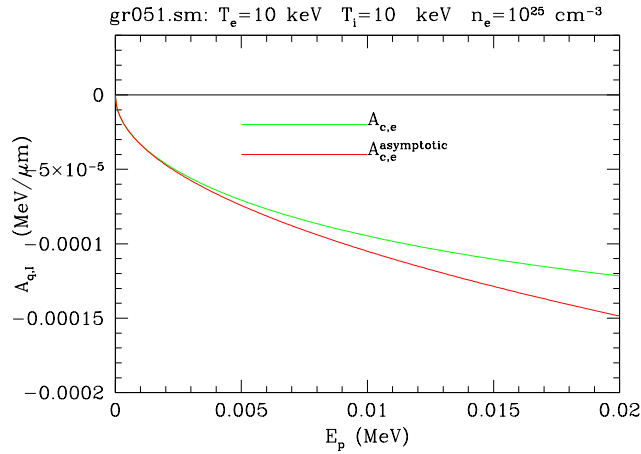


FIG. 6: Asymptotic quantum ion contribution at low energies. [gr001.f90, gr051.sm, gr001.dat, gr001.smallE.dat, gr051.eps]

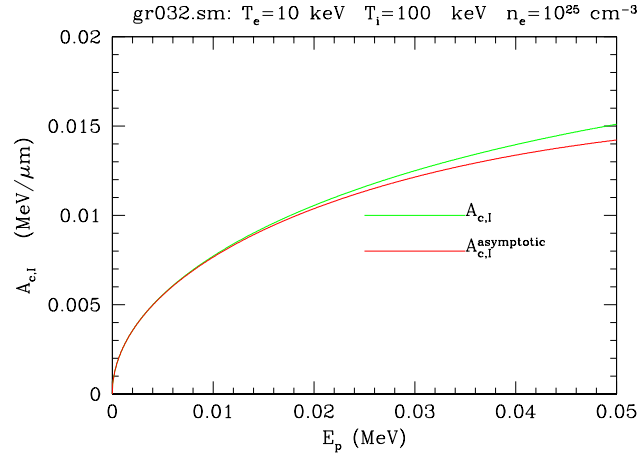
2. Temperatures $T_e = 10$ keV and $T_i = 100$ keV

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

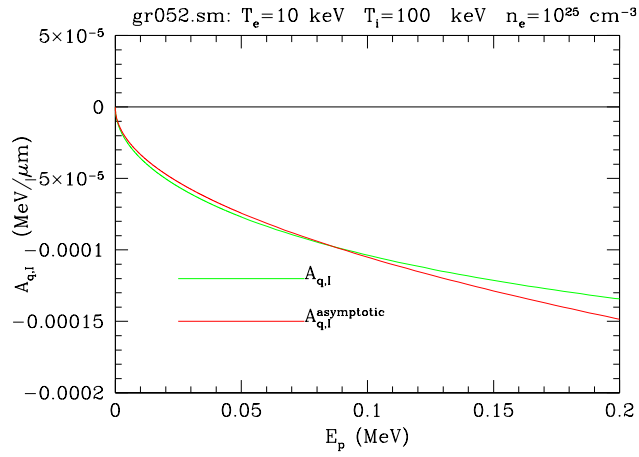


FIG. 8: Asymptotic quantum ion contribution at low energies. [gr002.f90, gr052.sm, gr002.dat, gr002.smallE.dat, gr052.eps]

3. Temperatures $T_e = 100 \text{ keV}$ and $T_i = 10 \text{ keV}$

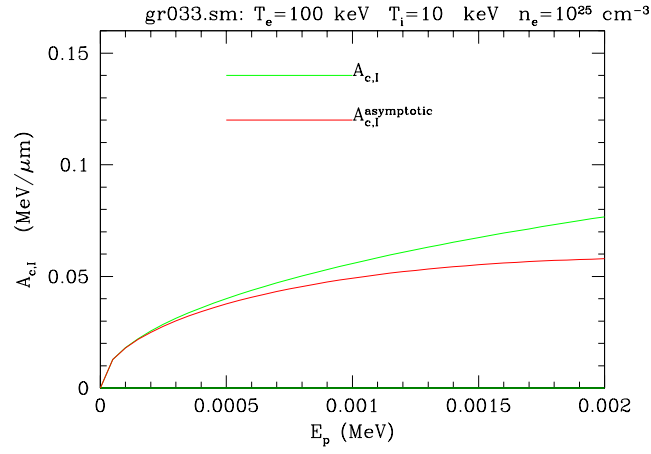


FIG. 9: Asymptotic classical ion contribution at low energies. [gr003.f90, gr033.sm, gr003.dat, gr003.smallE.dat, gr033.eps]

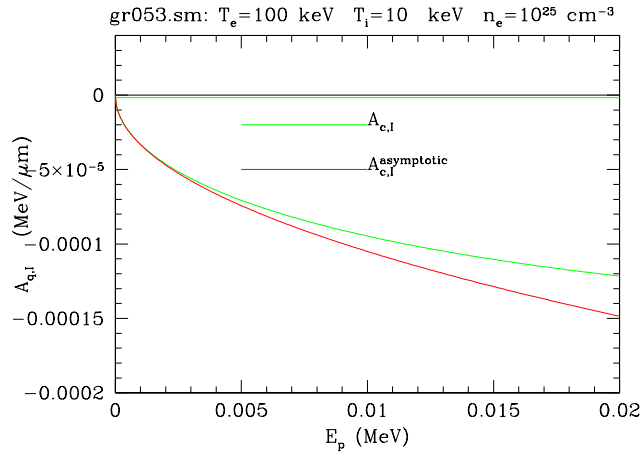


FIG. 10: Asymptotic quantum ion contribution at low energies. [gr003.f90, gr053.sm, gr003.dat, gr003.smallE.dat, gr053.eps]

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 $T_e = 10 \text{ keV}$ and $T_i = 10 \text{ keV}$

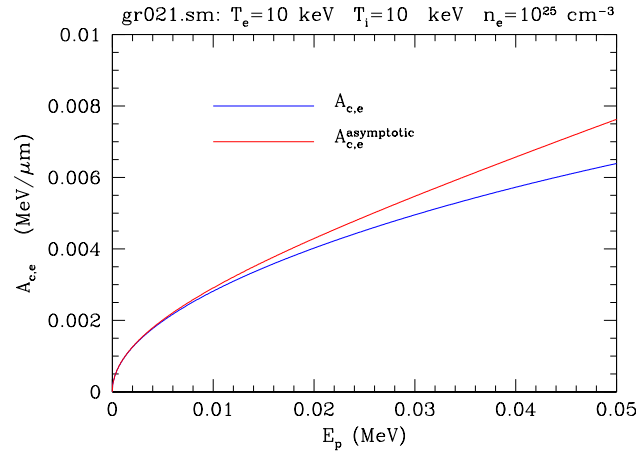


FIG. 11: Asymptotic classical electron contribution at low energies. [gr001.f90, gr021.sm, gr001.dat, gr001.smallE.dat, gr021.eps]

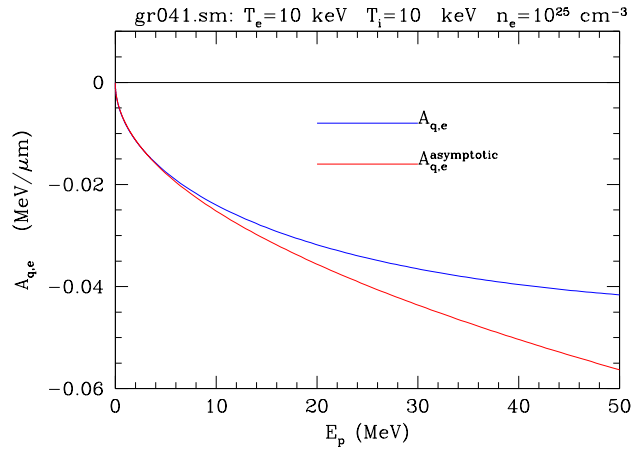


FIG. 12: Asymptotic quantum electron contribution at low energies. [gr001.f90, gr041.sm, gr001.dat, gr001.smallE.dat, gr041.eps]

2. Temperatures $T_e = 10 \text{ keV}$ and $T_i = 100 \text{ keV}$

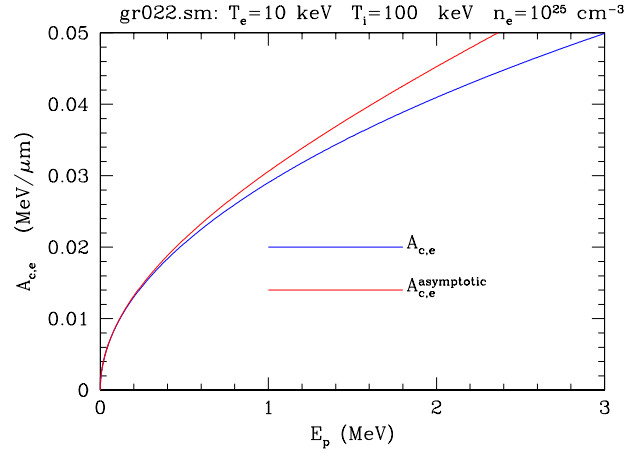


FIG. 13: Asymptotic classical electron contribution at low energies. [gr002.f90, gr022.sm, gr002.dat, gr002.smallE.dat, gr022.eps]

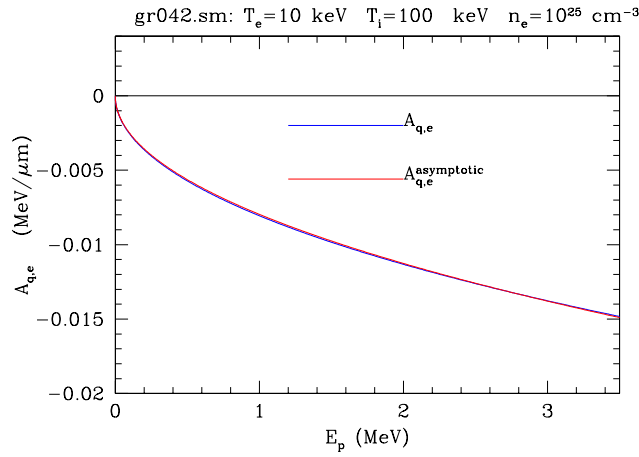


FIG. 14: Asymptotic quantum electron contribution at low energies. [gr002.f90, gr042.sm, gr002.dat, gr002.smallE.dat, gr042.eps]

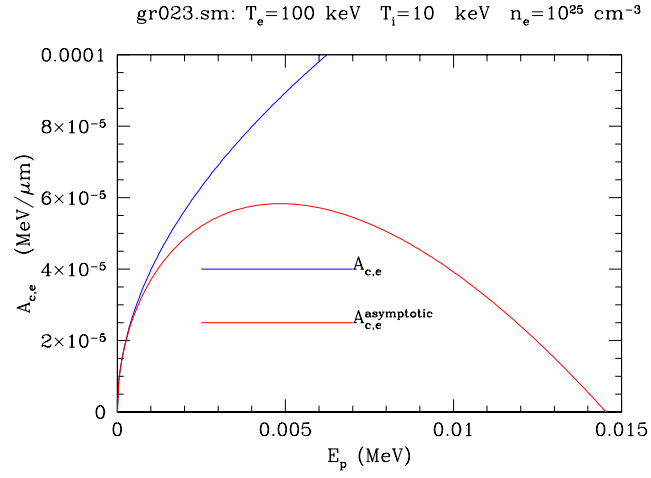
3. Temperatures $T_e = 100$ keV and $T_i = 10$ keV

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

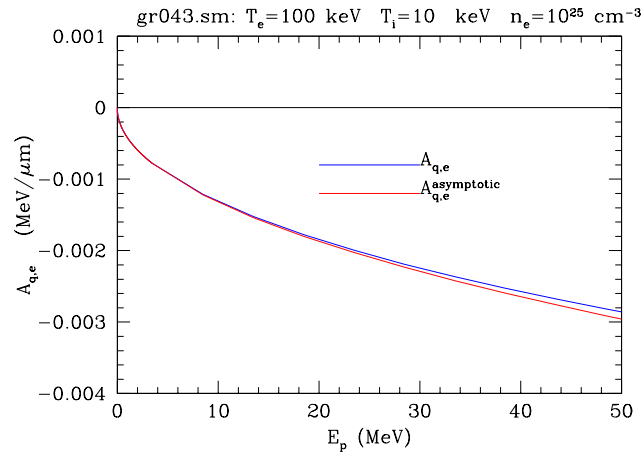


FIG. 16: Asymptotic quantum electron contribution at low energies. [gr003.f90, gr043.sm, gr003.dat, gr003.smallE.dat, gr043.eps]

C. Total Electron and Ion Contributions

1. Temperatures $T_e = 10$ keV and $T_i = 10$ keV

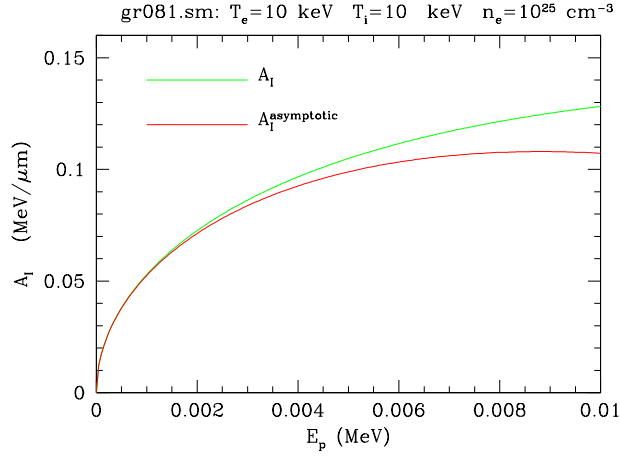


FIG. 17: Total asymptotic ion contribution at low energies. [gr001.f90, gr081.sm, gr001.dat, gr001.smallE.dat, gr081.eps]

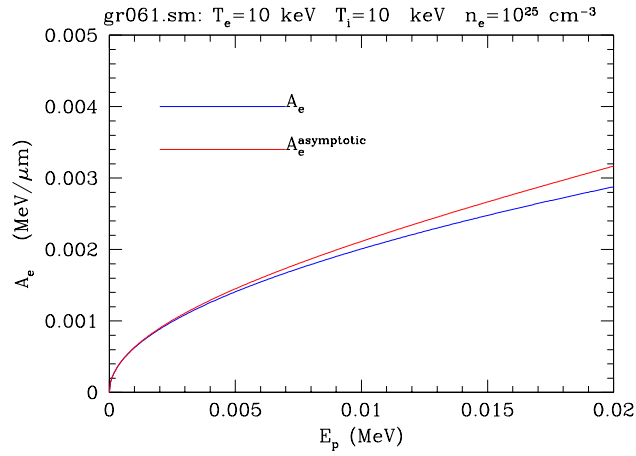


FIG. 18: Total asymptotic electron contribution at low energies. [gr001.f90, gr061.sm, gr001.dat, gr001.smallE.dat, gr061.eps]

2. Temperatures $T_e = 10$ keV and $T_i = 100$ keV

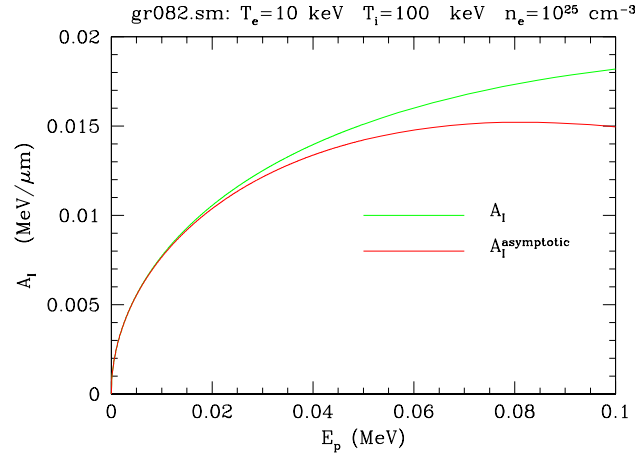


FIG. 19: Total asymptotic ion contribution at low energies. [gr002.f90, gr082.sm, gr002.dat, gr002.smallE.dat, gr082.eps]

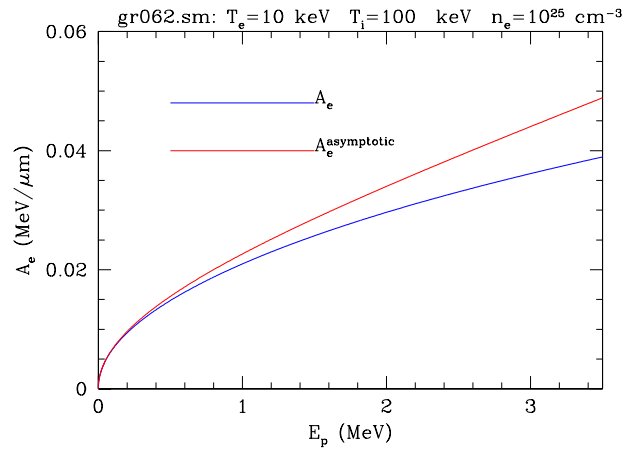


FIG. 20: Total asymptotic electron contribution at low energies. [gr002.f90, gr062.sm, gr002.dat, gr002.smallE.dat, gr062.eps]

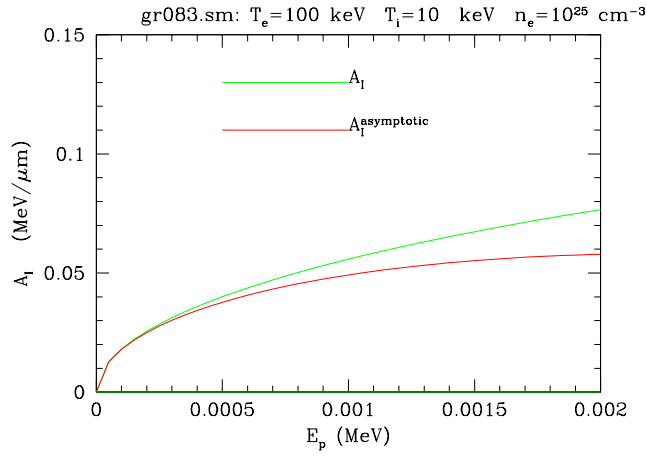
3. Temperatures $T_e = 100$ keV and $T_i = 10$ keV

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

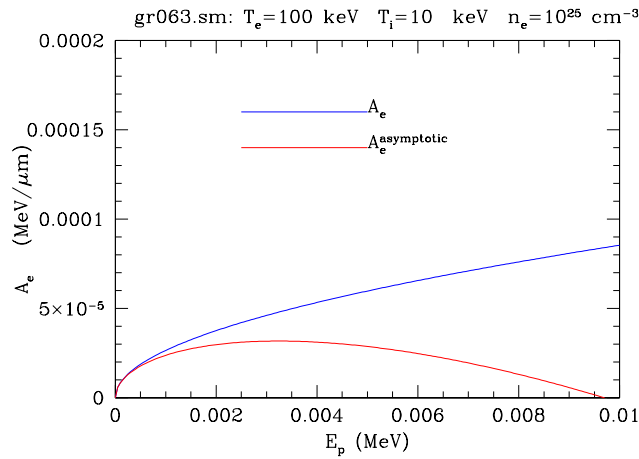


FIG. 22: Total asymptotic electron contribution at low energies. [gr003.f90, gr063.sm, gr003.dat, gr003.smallE.dat, gr063.eps]

D. More Classical: The Singular and Regular Contributions

Up to now, we have not been dividing the classical piece into its singular and regular contributions.

$$v_p \rightarrow 0 : \mathcal{A}_b(v_p) = \underbrace{\frac{e_p^2 \kappa_b^2}{4\pi}}_{c_1} \underbrace{\left(\frac{\beta_b m_b}{2\pi} \right)^{1/2}}_{c_2} v_p \cdot \left\{ \left(\bar{A}_{b,s}^{\text{CL}} + \bar{A}_{b,r}^< \right) + A_b^{\Delta Q} \right\}, \quad (2.6)$$

Since the code calculates the singular and regular pieces separately, let's explore their respective small energy asymptotics. These are given by Eq. (9.8) on p. 300 and Eq. (7.34) on p (287) of BPS, respectively:

$$\bar{A}_{b,s}^{\text{CL}} = - \left(\frac{2}{3} - \frac{1}{5} \beta_b m_b v_p^2 \right) \left[\ln \left\{ \frac{e_p e_b \beta_b K}{16\pi} \frac{m_b}{m_{pb}} \right\} + 2\gamma \right] + \frac{2}{15} \beta_b m_b v_p^2 + \mathcal{O}(v_p^4); \quad (2.7)$$

$$\begin{aligned} \bar{A}_{b,r}^< = - \left(\frac{2}{3} - \frac{1}{5} \beta_b m_b v_p^2 \right) \left[\frac{1}{2} + \ln \left\{ \frac{\kappa_D}{K} \right\} \right] + \frac{1}{5} \sum_c \frac{\kappa_c^2}{\kappa_D^2} \beta_c m_c v_p^2 - \\ \frac{\pi}{36} \left[\sum_c \frac{\kappa_c^2}{\kappa_D^2} (\beta_c m_c v_p^2)^{1/2} \right]^2 + \mathcal{O}(v_p^4). \end{aligned} \quad (2.8)$$

$$(2.9)$$

To leading order in v_p these expressions become,

$$\bar{A}_{b,s}^{\text{CL}} = -\frac{2}{3} \left[\ln \left\{ \frac{e_p e_b \beta_b K}{16\pi} \frac{m_b}{m_{pb}} \right\} + 2\gamma \right] + \mathcal{O}(v_p^2) \quad (2.10)$$

$$\bar{A}_{b,r}^< = -\frac{2}{3} \left[\frac{1}{2} + \ln \left\{ \frac{\kappa_D}{K} \right\} \right] + \mathcal{O}(v_p^2), \quad (2.11)$$

and upon adding them the K 's cancel and we return to (2.2). Keep the v_p^2 terms, we have the more precise expression (this is the one actually used in the code):

$$\bar{A}_{b,s}^{\text{CL}} = - \left(\frac{2}{3} - \frac{1}{5} \beta_b m_b v_p^2 \right) \left[\ln \left\{ \frac{e_p e_b \beta_b K}{16\pi} \frac{m_b}{m_{pb}} \right\} + 2\gamma \right] + \frac{2}{15} \beta_b m_b v_p^2 + \mathcal{O}(v_p^4) \quad (2.12)$$

$$\begin{aligned} \bar{A}_{b,r}^< = - \left(\frac{2}{3} - \frac{1}{5} \beta_b m_b v_p^2 \right) \left[\frac{1}{2} + \ln \left\{ \frac{\kappa_D}{K} \right\} \right] + \frac{1}{5} \sum_c \frac{\kappa_c^2}{\kappa_D^2} \beta_c m_c v_p^2 - \\ \frac{\pi}{36} \left[\sum_c \frac{\kappa_c^2}{\kappa_D^2} (\beta_c m_c v_p^2)^{1/2} \right]^2 + \mathcal{O}(v_p^4), \end{aligned} \quad (2.13)$$

$$\begin{aligned} \bar{A}_b^{\text{CL}} = \bar{A}_{b,s}^{\text{CL}} + \bar{A}_{b,r}^< = - \left(\frac{2}{3} - \frac{1}{5} \beta_b m_b v_p^2 \right) \left[\ln \left\{ \frac{e_p e_b \beta_b \kappa_D}{16\pi} \frac{m_b}{m_{pb}} \right\} + \frac{1}{2} + 2\gamma \right] + \frac{2}{15} \beta_b m_b v_p^2 \\ \frac{\pi}{36} \left[\sum_c \frac{\kappa_c^2}{\kappa_D^2} (\beta_c m_c v_p^2)^{1/2} \right]^2 + \mathcal{O}(v_p^4). \end{aligned} \quad (2.14)$$

1. Temperatures $T_e = 10 \text{ keV}$ and $T_i = 10 \text{ keV}$

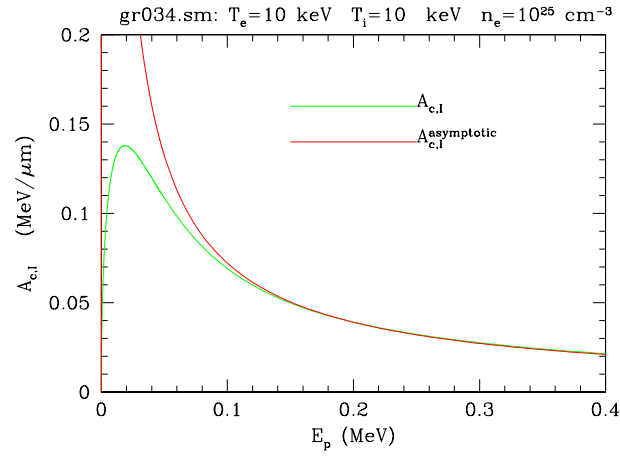


FIG. 23: Asymptotic singular ion contribution at low energies. [gr004.f90, gr004.dat, gr004.smallE.dat, gr104.sm]

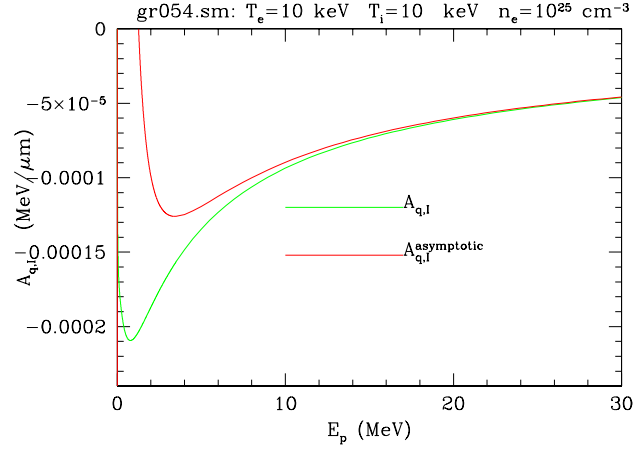


FIG. 24: Asymptotic regular ion contribution at low energies. *** [gr001.f90, gr034.sm, gr001.dat, gr001.highE.dat, gr034.eps] ***

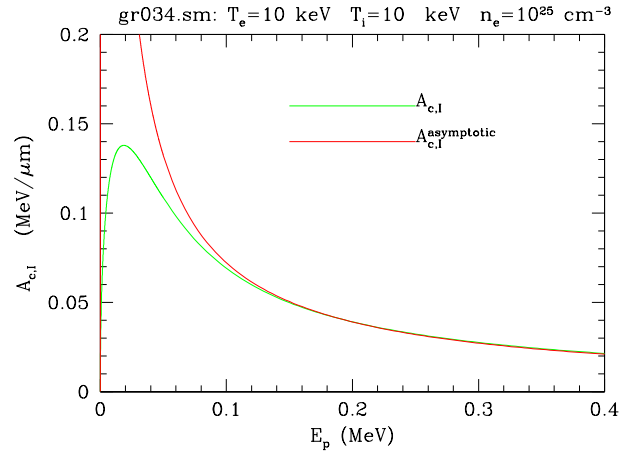


FIG. 25: Asymptotic singular electron contribution at low energies. *** [gr001.f90, gr034.sm, gr001.dat, gr001.highE.dat, gr034.eps] ***

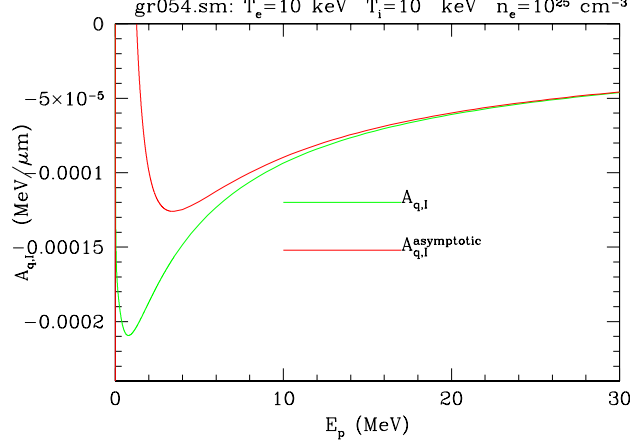


FIG. 26: Asymptotic regular electron contribution at low energies. *** [gr001.f90, gr034.sm, gr001.dat, gr001.highE.dat, gr034.eps] ***

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

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

$$\mathcal{A}_i^{\text{QM}} = \frac{e_p^2}{4\pi} \frac{1}{v_p^2} \sum_i \omega_i^2 \left[-\ln \left\{ \frac{\hbar \kappa_e}{2m_{pi} v_p} \right\} - \frac{1}{2} \right]. \quad (3.2)$$

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

$$E_p \gg T \quad \eta_{pi} = \frac{e_p e_i}{4\pi \hbar v_p} \gg 1 : \\ \mathcal{A}_{i,s}^C = -\frac{e_p^2}{4\pi} \frac{\omega_i^2}{v_p^2} \left[\ln \left\{ \frac{e_p e_i}{16\pi} \frac{2\kappa_e}{m_{pi} v_p^2} \right\} + \gamma \right] \quad [(\text{B40}) \text{ in text}] \quad (3.3)$$

The regular high energy asymptotic ion term is

$$E_p \gg T \quad \ln \left\{ \frac{m_i T_e^3}{m_e T_i^3} \right\} \\ \mathcal{A}_{i,R}^C = -\frac{e_p^2}{4\pi} \frac{\omega_i^2}{2v_p^2} \quad [(\text{B34}) \text{ in text w/o sum}] . \quad (3.4)$$

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

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

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

The algebra is:

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

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

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

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

1. Temperatures $T_e = 10 \text{ keV}$ and $T_i = 10 \text{ keV}$

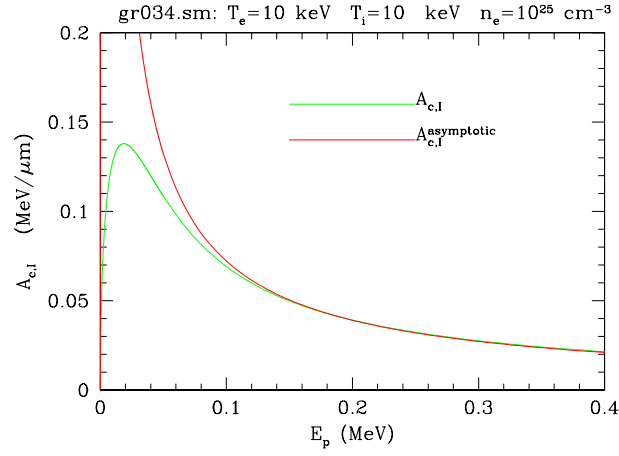


FIG. 27: Asymptotic classical ion contribution at high energies. [gr001.f90, gr034.sm, gr001.dat, gr001.highE.dat, gr034.eps]

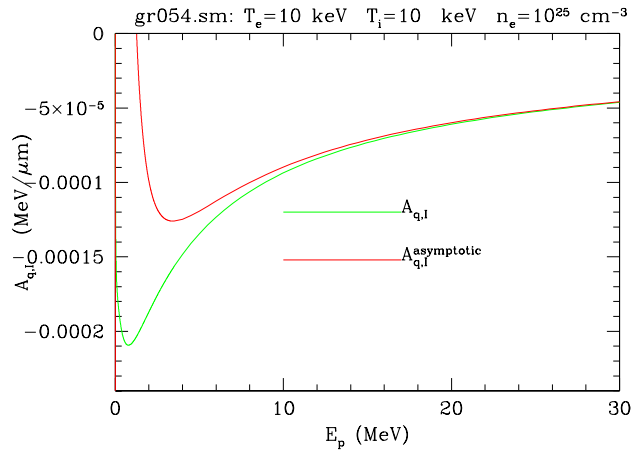


FIG. 28: Asymptotic quantum ion contribution at high energies. [gr001.f90, gr054.sm, gr001.dat, gr001.highE.dat, gr054.eps]

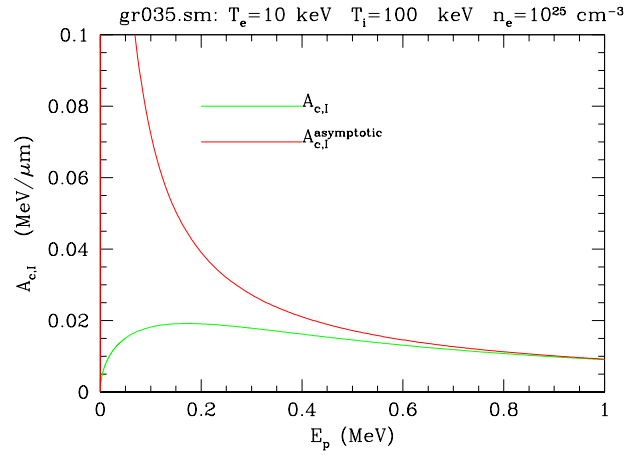
2. Temperatures $T_e = 10$ keV and $T_i = 100$ keV

FIG. 29: Asymptotic classical ion contribution at high energies. [gr002.f90, gr035.sm, gr002.dat, gr002.highE.dat, gr035.eps]

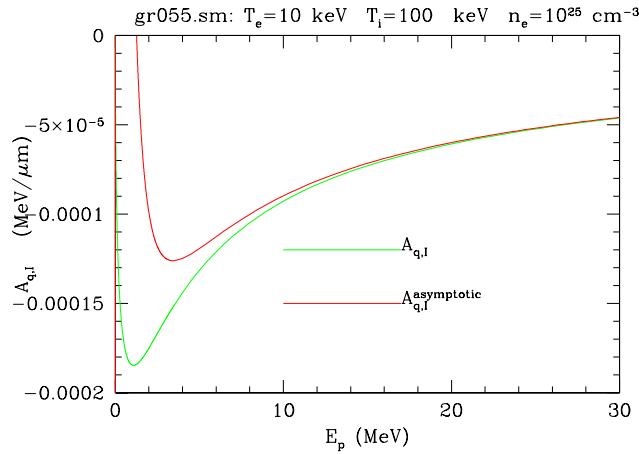


FIG. 30: Asymptotic quantum ion contribution at high energies. [gr002.f90, gr055.sm, gr002.dat, gr002.highE.dat, gr055.eps]

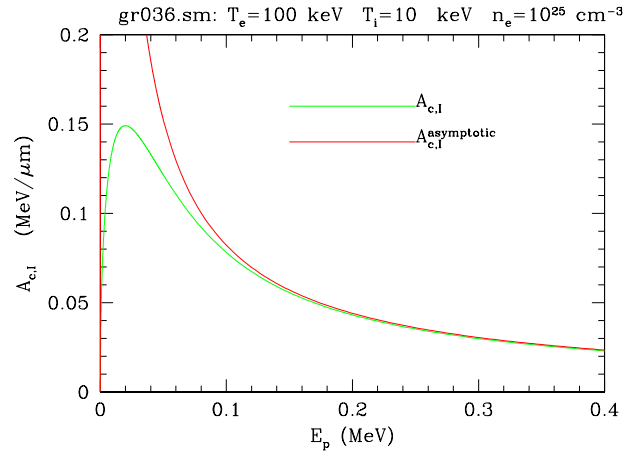
3. Temperatures $T_e = 100 \text{ keV}$ and $T_i = 10 \text{ keV}$ 

FIG. 31: Asymptotic classical ion contribution at high energies. [gr003.f90, gr036.sm, gr003.dat, gr003.highE.dat, gr036.eps]

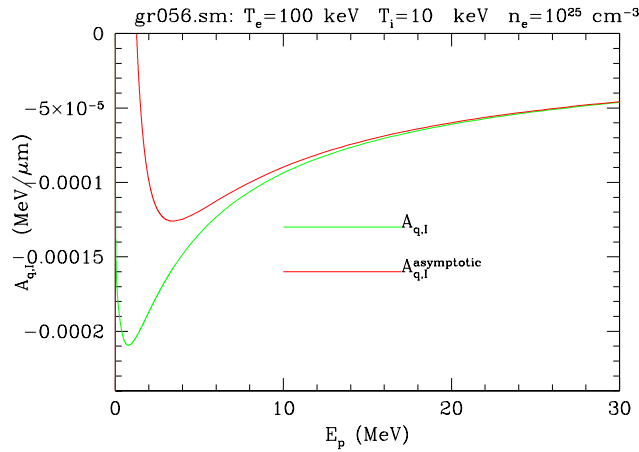


FIG. 32: Asymptotic quantum ion contribution at high energies. [gr003.f90, gr056.sm, gr003.dat, gr003.highE.dat, gr056.eps]

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 $m_i T / m_e$. In the high-intermediate energy regime,

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

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

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

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

and in the extreme high energy regime,

$$\begin{aligned} E_p &\gg \frac{m_i}{m_e} T : \\ \mathcal{A}_e &= \frac{e_p^2}{4\pi} \frac{\omega_e^2}{v_p^2} \ln \left\{ \frac{2m_{pe} v_p^2}{\hbar \omega_e} \right\} \quad [\text{(B58) in text}]. \end{aligned} \quad (3.13)$$

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

I will use the coding notation:

$$a_b = \frac{1}{2} \beta_b m_b v_p^2 = \frac{1}{2} \beta_b m_b c^2 (v_p^2 / c^2) \quad (3.14)$$

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

$$c_1 = \frac{e_p^2 \kappa_e^2}{4\pi} = Z_p^2 \cdot \frac{e^2}{8\pi a_0} \cdot 2a_0 \cdot \kappa_e^2 = 2Z_p^2 B_e \kappa_e^2 a_0. \quad (3.16)$$

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

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

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

and the intermediate high energy form is

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

1. *Temperatures $T_e = 10$ keV and $T_I = 10$ keV*

FIG. 33: Asymptotic classical electron contribution at high energies. [gr001.f90, gr024.sm, gr001.dat, gr001.highE.dat, gr024.eps]

FIG. 34: Asymptotic quantum electron contribution at high energies. [gr001.f90, gr044.sm, gr001.dat, gr001.highE.dat, gr044.eps]

2. *Temperatures $T_e = 10$ keV and $T_I = 100$ keV*

FIG. 35: Asymptotic classical electron contribution at high energies. [gr002.f90, gr025.sm, gr002.dat, gr002.highE.dat, gr025.eps]

FIG. 36: Asymptotic quantum electron contribution at high energies. [gr002.f90, gr045.sm, gr002.dat, gr002.highE.dat, gr045.eps]

3. *Temperatures $T_e = 100$ keV and $T_I = 10$ keV*

FIG. 37: Asymptotic classical electron contribution at high energies. [gr003.f90, gr026.sm, gr003.dat, gr003.highE.dat, gr026.eps]

FIG. 38: 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 $T_e = 10$ keV and $T_i = 10$ keV

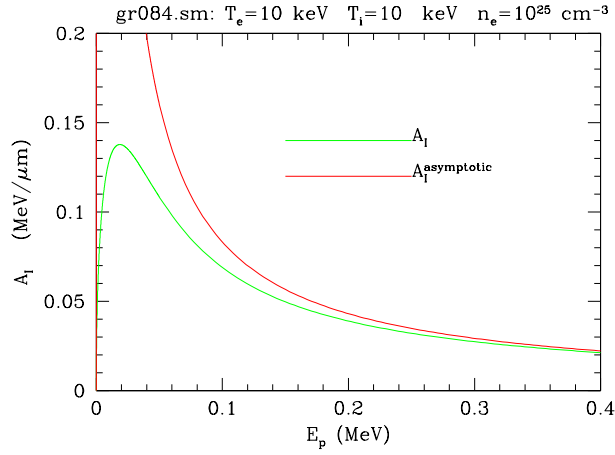


FIG. 39: Total asymptotic ion contribution at high energies. [gr001.f90, gr084.sm, gr001.dat, gr001.highE.dat, gr084.eps]

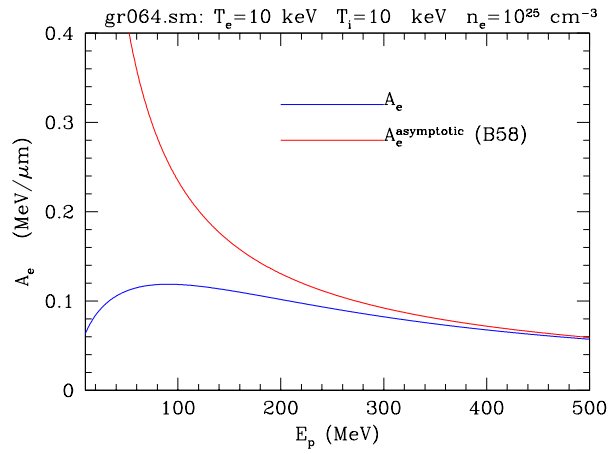


FIG. 40: Total asymptotic electron contribution (B58) at very high energies. [gr001.f90, gr064.sm, gr001.dat, gr001.very.highE.dat, gr064.eps]

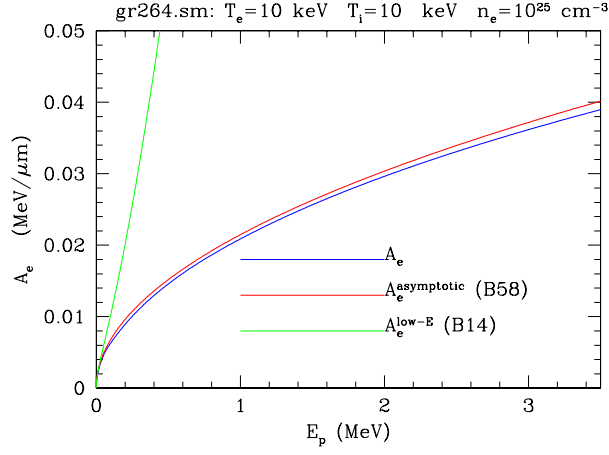


FIG. 41: Total asymptotic electron contribution (B56) at medium high energies. [gr001.f90, gr264.sm, gr001.dat, gr001.highE.dat, gr264.eps]

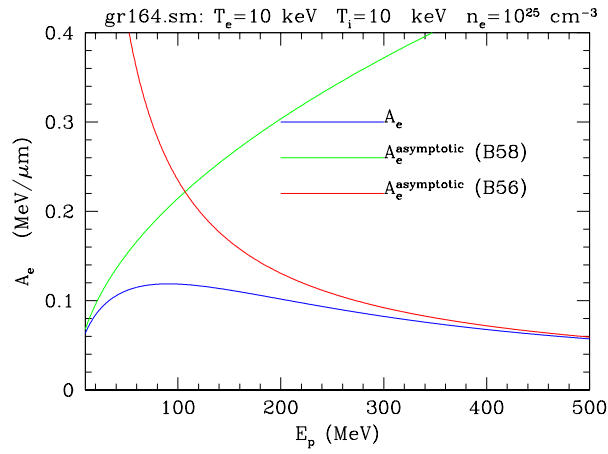


FIG. 42: Total asymptotic electron contribution (B56) and (B58). [gr001.f90, gr164.sm, gr001.dat, gr001.highE.dat, gr001.very.highE.dat, gr164.eps]

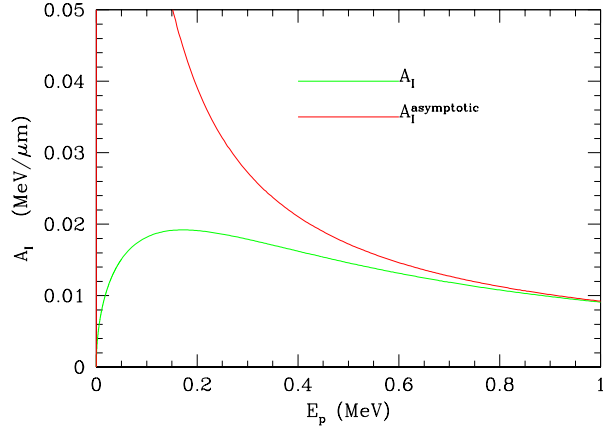
2. Temperatures $T_e = 10$ keV and $T_i = 100$ keVgr085.sm: $T_e = 10$ keV $T_i = 100$ keV $n_e = 10^{25}$ cm⁻³

FIG. 43: Total asymptotic ion contribution at high energies. [gr002.f90, gr085.sm, gr002.dat, gr002.highE.dat, gr085.eps]

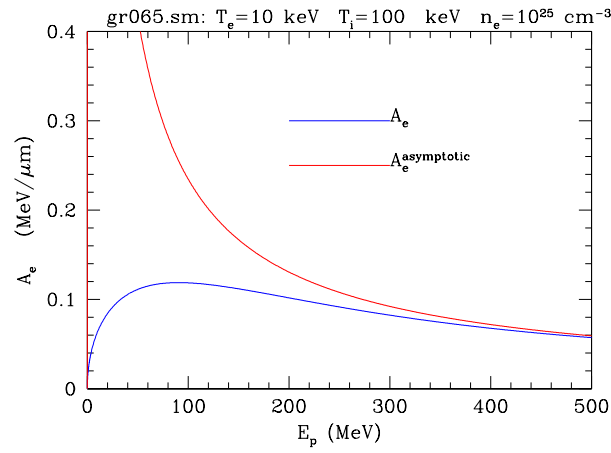


FIG. 44: Total asymptotic electron contribution (B58) at very high energies. [gr002.f90, gr065.sm, gr002.dat, gr002.highE.dat, gr065.eps]

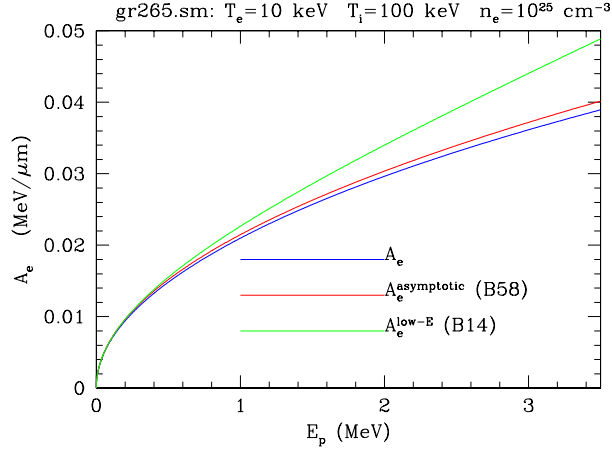


FIG. 45: Total asymptotic electron contribution (B56) at medium high energies. [gr002.f90, gr265.sm, gr002.dat, gr002.highE.dat, gr265.eps]

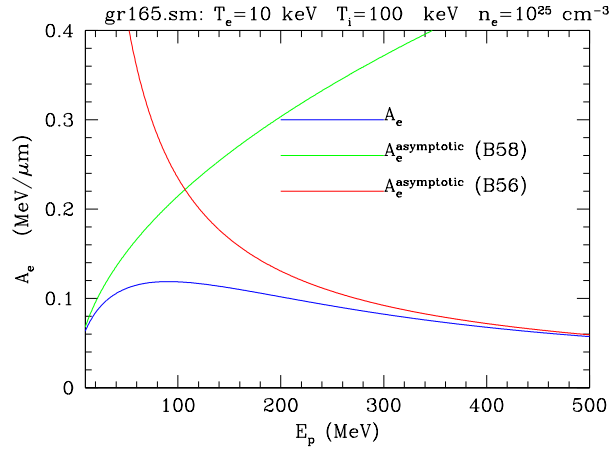


FIG. 46: Total asymptotic electron contribution (B56) and (B58). [gr002.f90, gr165.sm, gr002.dat, gr002.highE.dat, gr002.very.highE.dat, gr165.eps]

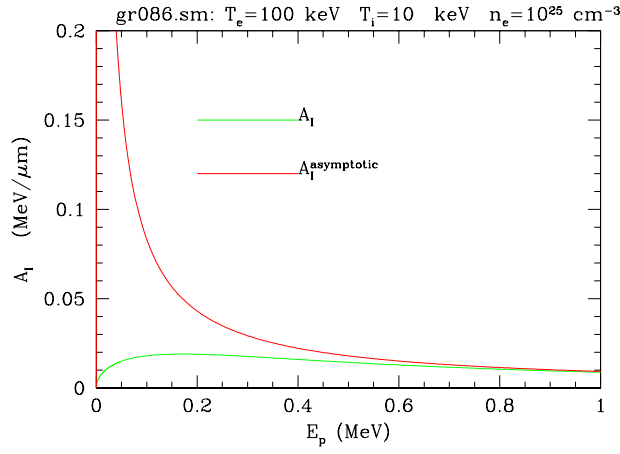
3. Temperatures $T_e = 100$ keV and $T_i = 10$ keV

FIG. 47: Total asymptotic ion contribution at high energies. [gr003.f90, gr086.sm, gr003.dat, gr003.highE.dat, gr086.eps]

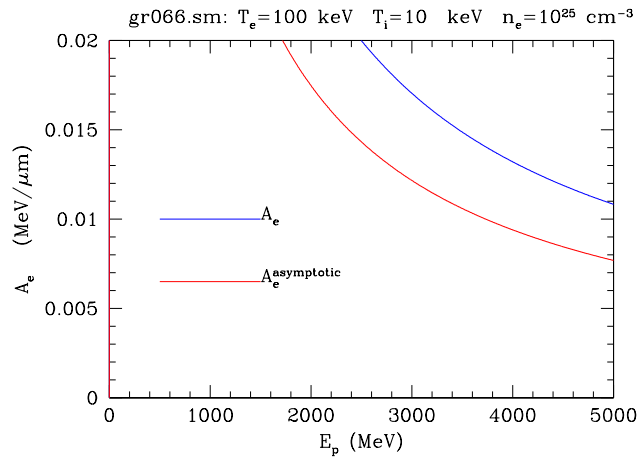


FIG. 48: Total asymptotic electron contribution (B58) at very high energies. [gr003.f90, gr066.sm, gr003.dat, gr003.very.highE.dat, gr066.eps]

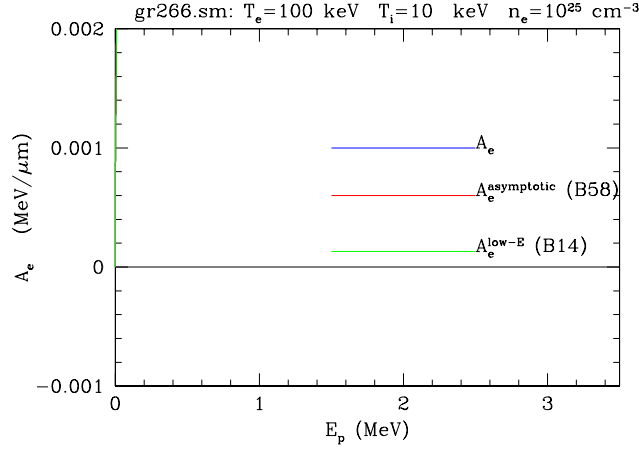


FIG. 49: Total asymptotic electron contribution (B56) at medium high energies. [gr003.f90, gr266.sm, gr003.dat, gr003.highE.dat, gr266.eps]

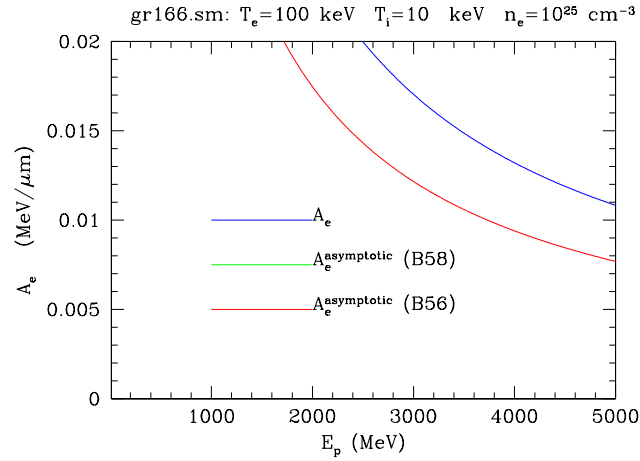


FIG. 50: Total asymptotic electron contribution (B56) at medium high energies. [gr003.f90, gr166.sm, gr003.dat, gr003.highE.dat, gr003.very.highE.dat, gr166.eps]

Appendix A: Coding the A-coefficients

1. The Singular Contribution

The singular contribution,

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

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

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

which motivates the definition

$$\mathcal{A}_{b,s}^C = c_{b,1} c_{b,2} \cdot \mathcal{A}_s(a_{pb}, b_{pb}) \quad (\text{A3})$$

$$\mathcal{A}_s(a, b) = \int_0^1 du u^{1/2} e^{-a u} \left[-\ln \left\{ \frac{u}{1-u} \right\} + b \right] \quad (\text{A4})$$

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

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

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

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

$$= \frac{e_p^2}{4\pi} \frac{i}{2\pi} \int_0^1 du u \frac{\rho_b(v_p u)}{\rho_{\text{total}}(v_p u)} \left[F(v_p u) \ln \left\{ \frac{F(v_p u)}{K^2} \right\} - F^*(v_p u) \ln \left\{ \frac{F^*(v_p u)}{K^2} \right\} \right] \quad (\text{A8})$$

$$= -\frac{e_p^2}{4\pi} \frac{1}{2\pi} \int_0^1 du u \frac{\rho_b(v_p u)}{\rho_{\text{total}}(v_p u)} H(v_p u) , \quad (\text{A9})$$

where we have defined

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

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

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

Defining the parameters

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

$$\bar{\kappa}_c^2 \equiv \frac{\kappa_c^2}{K^2} \quad (\text{A13})$$

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

$$\mathbb{F}_{\text{Re}}(\{a_c v\}, \{\bar{\kappa}_c\}) = \sum_c \bar{\kappa}_c^2 \left(1 - 2a_c v \operatorname{daw}\{a_c v\} \right) \quad (\text{A14})$$

$$\mathbb{F}_{\text{Im}}(\{a_c v\}, \{\bar{\kappa}_c\}) = \sqrt{\pi} \sum_c \bar{\kappa}_c^2 a_c v e^{-a_c^2 v^2} . \quad (\text{A15})$$

The ratio of weighting factors can be written

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

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

or

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

We can now express the regular piece as

$$\mathcal{A}_{b,R}^C = \underbrace{\left[\frac{e_p^2 \kappa_b^2}{4\pi} \right]}_{c_{b,1}} \cdot A_R(v_p, \{a_c\}, \{\bar{\kappa}_c\}) \quad (\text{A19})$$

$$A_{b,R}(v_p, \{a_c\}, \{\bar{\kappa}_c\}) = \int_0^1 du \underbrace{\mathbb{R}_b(\{a_c v_p u\}) \mathbb{H}(\{a_c v_p u\}, \{\bar{\kappa}_c\})}_{\text{dab_reg}}. \quad (\text{A20})$$

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 [cm/s]
INTEGER,                             INTENT(IN)  :: ib          ! Species number
INTEGER,                             INTENT(IN)  :: nni         ! Number of ion species
REAL,                                INTENT(IN)  :: k2           ! Wavenumber squared [1/km]
REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: kb2           ! Debye wavenumber squared [1/km]
REAL,    DIMENSION(1:nni+1), INTENT(IN)  :: betab          ! Temperature array [1/km]
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=0.55555555556E0, W2=0.88888888889E0
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

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

The quantum function we need to code is therefore

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

where the arguments of the function are defined by

$$a_{pb} = \frac{1}{2} \beta_b m_b v_p^2 \quad (\text{A23})$$

$$\begin{aligned} \tilde{\eta}_{pb} &= \frac{e_p e_b}{4\pi \hbar v_p} = |Z_p Z_b| \frac{e^2}{8\pi a_0} \frac{2a_0}{\hbar} \frac{1}{v_p} = |Z_p Z_b| \cdot 13.606 \text{ eV} \cdot \frac{2 \cdot 5.29 \times 10^{-9} \text{ cm}}{6.5821 \times 10^{-16} \text{ eV s}} \frac{1}{v_p} \\ &= 2.1870 \times 10^8 \frac{|Z_p Z_b|}{v_p \cdot (\text{cm/s})^{-1}}, \end{aligned} \quad (\text{A24})$$

and the function itself takes the form

$$\begin{aligned} \mathbf{A}_1^{\text{QM}}(a, \eta) &= - \int_0^\infty du \left[\text{Re} \psi \left\{ 1 + i \frac{\eta}{u} \right\} - \ln \left\{ \frac{\eta}{u} \right\} \right] \\ &\quad \frac{1}{2a u} \left[\left(e^{-a(u-1)^2} + e^{-a(u+1)^2} \right) - \frac{e^{-a(u-1)^2} - e^{-a(u+1)^2}}{2a u} \right]. \end{aligned} \quad (\text{A25})$$

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 $T \ll E_p \ll (m_i/m_e) T$ and an extreme high energy regime $E \gg (m_i/m_e) T$.

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 $\mathcal{A}_{e,s}^c$ and $\mathcal{A}_{e,r}^<$ respectively. The quantum asymptotic correction can then be obtained by

$$\mathcal{A}_e^{\text{QM}} = \mathcal{A}_e - \mathcal{A}_e^c = \mathcal{A}_e - (\mathcal{A}_{e,s}^c + \mathcal{A}_{e,r}^<).$$

Before coeff_bps_high_E returns the same quantities for electrons and ions, I will need to analytically calculate $\mathcal{A}_{e,s}^c$ and $\mathcal{A}_{e,r}^<$ 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}_i .

1. The A-Coefficients

acoeff.f90:

```
!
! Robert Singleton
! - Santa Fe, Winter 2005
! - Santa Fe, March 2009 [start rewrite]
! - Santa Fe, November 2009 [finish rewrite]
!
!
! 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 ( $g \ll 1$ ),
! 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.  $mp = mp[\text{grams}] \cdot c^2$ 
!
! 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  $T_e \neq T_I$ . 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  $g = e^2 \kappa / (4\pi T)$ ; 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  $g \ll 1$ , 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 ( $\eta \ll 1$  means
! extreme classical scattering while  $\eta \gg 1$  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  $\eta = e^2 / (4\pi \hbar v_{\text{thermal}})$ 
! (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 ( $g \gg 1$ ), 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]
!
! 
$$= c \sqrt{\frac{2 E_p}{m_p c^2}}$$

! where  $m_p$  and  $E_p$  are in keV and
!  $c$  is the speed of light in cm/s
!
! 
$$c_1 = \frac{e^2 k_b^2}{4 \pi} = 2 z_p^2 * B_e * k_b^2 * a_0$$

! [keV/cm]
! [MeV/micron]
!
! 
$$c_2 = \left[ \frac{\beta_{\text{tab}} m_b c^2}{2 \pi} \right]^{1/2} \frac{vp}{[dimensionless]}$$

!
! 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
INTEGER,                                INTENT(IN)  :: nni      ! Plasma:
REAL,                                   INTENT(IN)  :: ep       ! number of ions
REAL,                                   INTENT(IN)  :: mp       ! energy input [keV]
REAL,                                   INTENT(IN)  :: zp       ! mass [keV]
REAL,                                   INTENT(IN)  :: ia       ! charge
REAL,                                   INTENT(IN)  :: ib       !
REAL,                                   INTENT(IN)  :: betab    ! temp array [1/keV]
INTEGER,                                INTENT(IN)  :: mb       ! mass array [keV]
INTEGER,                                INTENT(IN)  :: nb       ! density [1/cc]
REAL,    DIMENSION(1:nni+1),           INTENT(IN)  :: zb       ! charge array
REAL,    DIMENSION(1:nni+1),           INTENT(IN)  ::          ! A-coeffs [MeV/micron]
REAL,    DIMENSION(1:nni+1),           INTENT(OUT) :: a_ab
REAL,    DIMENSION(1:nni+1),           INTENT(OUT) :: a_ab_sing
REAL,    DIMENSION(1:nni+1),           INTENT(OUT) :: a_ab_reg
REAL,    DIMENSION(1:nni+1),           INTENT(OUT) :: a_ab_qm

REAL,    DIMENSION(1:nni+1) :: mpb, mbpb, kb2, ab
REAL,    DIMENSION(1:nni+1) :: vp, zp2, k, k2, kd, kd2, a, b, eta
REAL,    DIMENSION(1:nni+1) :: 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*zp*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 ! [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
  INTEGER,                                INTENT(IN)    :: nni      ! Plasma:
  REAL,                                   INTENT(IN)    :: ep        ! number of ions
  REAL,                                   INTENT(IN)    :: betab     ! energy
  REAL,    DIMENSION(1:nni+1),           INTENT(IN)    :: zb       ! temp array [1/ke
  REAL,    DIMENSION(1:nni+1),           INTENT(IN)    :: mb       ! charge array
  REAL,    DIMENSION(1:nni+1),           INTENT(IN)    :: nb       ! mass array [keV]
  REAL,    DIMENSION(1:nni+1),           INTENT(IN)    ::          ! 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
INTEGER,          INTENT(IN)      :: nni      ! Plasma:
REAL,             DIMENSION(1:nni+1), INTENT(IN) :: betab ! number of ions
REAL,             DIMENSION(1:nni+1), INTENT(IN) :: mb   ! temp array [1/keV]
REAL,             DIMENSION(1:nni+1), INTENT(IN) :: nb   ! mass array [keV]
REAL,             DIMENSION(1:nni+1), INTENT(IN) :: zb   ! density [1/cc]
REAL,             DIMENSION(1:nni+1), INTENT(IN) :: zp   ! charge array
!
REAL,             INTENT(IN)      :: ep        ! Projectile
REAL,             INTENT(IN)      :: mp        ! projectile energy [keV]
REAL,             INTENT(IN)      :: zp        ! projectile mass [keV]
!
REAL,             INTENT(OUT)     :: a_tot     ! A-coeffs [MeV/micron]
REAL,             INTENT(OUT)     :: a_i       ! electron + ion
REAL,             INTENT(OUT)     :: a_e       ! ion contribution
REAL,             INTENT(OUT)     :: ac_tot    ! electron contribution
REAL,             INTENT(OUT)     :: ac_i      ! classical
REAL,             INTENT(OUT)     :: ac_e      ! classical
REAL,             INTENT(OUT)     :: aq_tot    ! classical
REAL,             INTENT(OUT)     :: aq_i      ! quantum
REAL,             INTENT(OUT)     :: aq_e      ! quantum
REAL,             INTENT(OUT)     :: ac_s_i    ! quantum
REAL,             INTENT(OUT)     :: ac_s_e    ! quantum
REAL,             INTENT(OUT)     :: ac_r_i    ! quantum

```

```

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
!
!      h=2*(fr*farg + fi*LOG(fabs))
!
! 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=0.55555555556E0, W2=0.88888888889E0
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.

$$\frac{dE_b}{dx}(vp) = \left[\begin{array}{c} 1 \\ 1 - \frac{1}{\beta_b m_p vp} \end{array} \right] \text{Sum}_l \frac{d}{d vp^l} \{ \hat{vp}^l A_b(vp) \}$$

$$= \left[\begin{array}{c} 2 T_b \\ 1 - \frac{2 T_b}{m_p vp^2} \end{array} \right] * A_b(vp) - \frac{T_b}{m_p vp} * \frac{dA_b}{dvp}(vp)$$

$$= \left[\begin{array}{c} T_b \\ 1 - \frac{T_b}{E_p} \end{array} \right] * A_b(E_p) - T_b * \frac{dA_b}{dE_p}(E_p)$$

```

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

```

```

  INTEGER, INTENT(IN) :: nni ! Plasma:
                                ! 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 contribution
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_e_p
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_e_m
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_e
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  $E_p \ll T$ : 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.  $mp = mp[\text{grams}] * c^2$ 
!
! 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 [ $\text{cm}^{-3}$ ].
!
! 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, ac_s_i_lim, ac_s_e_lim, &
    ac_r_i_lim, ac_r_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
REAL,      INTENT(IN)              :: ep          ! projectile energy [k
REAL,      INTENT(IN)              :: mp          ! projectile mass [k
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 contribution
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,      INTENT(OUT)             :: ac_s_i_lim  ! singular
REAL,      INTENT(OUT)             :: ac_s_e_lim  ! singular
REAL,      INTENT(OUT)             :: ac_r_i_lim  ! regular
REAL,      INTENT(OUT)             :: ac_r_e_lim  ! regular

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      :: vp                    ! [cm/s]
REAL      :: vp2                   ! [cm^2/s^2]
REAL      :: kd2                   ! [1/cm^2]
REAL      :: a, zp2                ! [dimensionless]
REAL      :: c1                    ! [keV/cm]
REAL      :: c2                    ! [dimensionless]

nnb = nni+1
vp  = CC*SQRT(2*ep/mp)              ! [cm/s]
vp2 = vp*vp                        ! [cm^2/s^2]
kb2 = DEBYE2*zp*zb*nb*betab        ! [1/cm^2]
kd2 = SUM(kb2)                     ! [1/cm^2]
zp2 = zp**2                         ! [dimensionless]
ab  = 0.5*betab*mb*vp2/CC2          ! [dimensionless]
                                         ! ab=(1/2) betab(ib)*mbc2(ib)*vp2/CC2

!
! 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
ac_s_i_lim = 0
ac_s_e_lim = 0
ac_r_i_lim = 0
ac_r_e_lim = 0
!
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
!

```

```

        CALL a_sing_ib_small_E(nni,ib,ep,zp,mp,betab,zb,mb,nb,ac_s_lim)
        ac_s_lim=c1*c2*ac_s_lim
!
! regular: asymptotic low energy form
!
        CALL a_reg_ib_small_E(nni,ib,ep,zp,mp,betab,zb,mb,nb,ac_r_lim)
        ac_r_lim=c1*ac_r_lim
!
! quantum: asymptotic low energy form
!
        CALL aq_ib_small_E(nni, ib, ep, zp, mp, betab, zb, mb, nb, aq_lim)
        aq_lim=c1*c2*aq_lim
!
! collect components
!
        CALL a_collect(ib,nnb,ac_s_lim,ac_r_lim,aq_lim,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,&
            ac_s_i_lim, ac_s_e_lim, ac_r_i_lim, ac_r_e_lim)
        ENDIF
        ENDDO
    END SUBROUTINE coeff_bps_small_E
!
! Same as coeff_bps_small_E, except returns A-coefficients for a single plasma
! index ib.
!

SUBROUTINE a_sing_ib_small_E(nni, ib, ep, zp, mp, betab, zb, mb, nb, ac_s_lim)
USE physvars
USE mathvars
IMPLICIT NONE
INTEGER,          INTENT(IN)  :: nni      ! number of ions
INTEGER,          INTENT(IN)  :: ib       ! plasma species number
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
REAL,             INTENT(IN)  :: ep       ! projectile energy [keV]
REAL,             INTENT(IN)  :: mp       ! projectile mass [ke]
REAL,             INTENT(IN)  :: zp       ! projectile charge
REAL,             INTENT(OUT) :: ac_s_lim ! A-coeffs [MeV/micron]

REAL,             DIMENSION(1:nni+1) :: kb2 ! [1/cm^2]
REAL,             DIMENSION(1:nni+1) :: ab  ! [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]

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]
!

```

```

      a=ab(ib)                                ! [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
!
      END SUBROUTINE a_sing_ib_small_E

SUBROUTINE a_reg_ib_small_E(nni, ib, ep, zp, mp, betab, zb, mb, nb, ac_r_lim)
USE physvars
USE mathvars
IMPLICIT NONE
INTEGER,                                INTENT(IN)  :: nni      ! number of ions
INTEGER,                                INTENT(IN)  :: ib       ! plasma species number
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
REAL,      INTENT(IN)  :: ep      ! projectile energy [keV]
REAL,      INTENT(IN)  :: mp      ! projectile mass [keV]
REAL,      INTENT(IN)  :: zp      ! projectile charge
REAL,      INTENT(OUT) :: ac_r_lim ! A-coeffs [MeV/micron]

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      :: ar1, ar2, c2        ! [dimensionless]

vp = CC*SQRT(2*ep/mp)           ! [cm/s]
vp2 = vp*vp                     ! [cm^2/s^2]
kb2 = DEBYE2*zp*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]
!
a=ab(ib)                        ! [dimensionless]
c2=SQRT(a/PI)                   ! [dimensionless]
!
! 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=-c2*((THIRD - 0.2*a)*(LOG(kd2/k2)+1) + ar1 + ar2 )
      END SUBROUTINE a_reg_ib_small_E

SUBROUTINE aq_ib_small_E(nni, ib, ep, zp, mp, betab, zb, mb, nb, aq_lim)
USE physvars

```

```

USE mathvars
IMPLICIT NONE
INTEGER,          INTENT(IN)  :: nni      ! number of ions
INTEGER,          INTENT(IN)  :: ib       ! plasma species number
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
REAL,             INTENT(IN)  :: ep       ! projectile energy [ke]
REAL,             INTENT(IN)  :: mp       ! projectile mass [ke]
REAL,             INTENT(IN)  :: zp       ! projectile charge
REAL,             INTENT(OUT) :: aq_lim  ! A-coeffs [MeV/micron]

REAL,             DIMENSION(1:nni+1) :: kb2 ! [1/cm^2]
REAL,             DIMENSION(1:nni+1) :: ab   ! [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 :: etbar, etbar2     ! [dimensionless]

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=(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]
!
! a=ab(ib)                 ! [dimensionless]
!
! 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
ELSE
  aq_lim=-1./(27*etbar2)
ENDIF
END SUBROUTINE aq_ib_small_E

```

3. 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  $E_p \gg T$ .
! For electrons there are two regimes:
! (i) extreme high energy  $E_p \gg (m_I/m_e)*T$  [coeff_bps_very_high_E]
! (ii) intermediate high energy  $T \ll E_p \ll (m_I/m_e)*T$  [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.  $mp = mp[\text{grams}] * c^2$ 
!
! 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 [ $\text{cm}^{-3}$ ].
!
! 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, ac_s_i_lim, ac_s_e_lim,      &
    ac_r_i_lim, ac_r_e_lim)
USE physvars
USE mathvars
IMPLICIT NONE
INTEGER,
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,          INTENT(OUT) :: ac_s_i_lim
REAL,          INTENT(OUT) :: ac_s_e_lim
REAL,          INTENT(OUT) :: ac_r_i_lim
REAL,          INTENT(OUT) :: ac_r_e_lim

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*zp*zp*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
ac_s_i_lim = 0
ac_s_e_lim = 0
ac_r_i_lim = 0
ac_r_e_lim = 0

!
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*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_i_lim, &
        a_e_lim,ac_tot_lim,ac_i_lim,ac_e_lim,aq_tot_lim,aq_i_lim,aq_e_lim, &
        ac_s_i_lim, ac_s_e_lim, ac_r_i_lim, ac_r_e_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, ac_s_i_lim, ac_s_e_lim, &
  ac_r_i_lim, ac_r_e_lim)
USE physvars
USE mathvars
IMPLICIT NONE
INTEGER,          DIMENSION(1:nni+1), 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,          INTENT(OUT) :: ac_s_i_lim
REAL,          INTENT(OUT) :: ac_s_e_lim
REAL,          INTENT(OUT) :: ac_r_i_lim
REAL,          INTENT(OUT) :: ac_r_e_lim

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
ac_s_i_lim=0
ac_s_e_lim=0

```

```

      ac_r_i_lim=0
      ac_r_e_lim=0
!
      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
!
! 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_i_lim,&
            a_e_lim,ac_tot_lim,ac_i_lim,ac_e_lim,aq_tot_lim,aq_i_lim,aq_e_lim,&
            ac_s_i_lim, ac_s_e_lim, ac_r_i_lim, ac_r_e_lim)
          ENDIF
        ENDDO
      END SUBROUTINE coeff_bps_very_high_E

```