

Clog Doc: ccoeff1.0.tex

C-Coefficient in Clog

Robert Singleton

Research Notes

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Robert L Singleton Jr

School of Mathematics

University of Leeds

LS2 9JT

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Abstract

Physics documentation for the BPS stopping power in the code Clog.

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I. GENERAL ANALYTIC EXPRESSIONS FOR THE BPS C-COEFFICIENTS

Suppose we have a plasma with various species labeled by an index b at distinct temperatures T_b , number densities n_b , and species masses m_b .¹ Temperature will be measured in energy units, and we denote the inverse temperature by $\beta_b = 1/T_b$. Electrostatic units will be rationalized cgs. The projectile will have mass m_a , charge e_a and energy $E_a = \frac{1}{2} m_a v_a^2$. The BPS $\mathcal{C}^{\ell\ell}$ -coefficients take the form

$$C_{ab}^{\ell\ell} = \left(C_{ab,R}^{\ell\ell<} + C_{ab,S}^{\ell\ell c} \right) + C_{ab}^{\ell\ell \Delta Q} \quad (1.1)$$

with

$$C_{ab,R}^{\ell\ell<} = \frac{e_a^2}{4\pi} \frac{1}{\beta_b v_a} \frac{i}{2\pi} \int_{-1}^1 \frac{d \cos \theta}{\cos \theta} \frac{\rho_b(v_a \cos \theta)}{\rho_{\text{total}}(v_a \cos \theta)} F(v_a \cos \theta) \ln \left\{ \frac{F(v_a \cos \theta)}{K^2} \right\}, \quad (1.2)$$

$$C_{ab,S}^{\ell\ell c} = \frac{e_a^2 \kappa_b^2}{4\pi} \left(\frac{\beta_b m_b v_a^2}{2\pi} \right)^{1/2} \frac{1}{\beta_b v_a} \int_0^1 du u^{-1/2} \exp \left\{ -\frac{1}{2} \beta_b m_b v_a^2 u \right\} \left[-\ln \left(\beta_b \frac{e_a e_b}{4\pi} K \frac{m_b}{m_{ab}} \frac{u}{1-u} \right) - 2\gamma \right] \quad (1.3)$$

$$C_{ab}^{\ell\ell \Delta Q} = -\frac{e_a^2 \kappa_b^2}{4\pi} \left(\frac{\beta_b m_b v_p^2}{2\pi} \right)^{1/2} \frac{1}{\beta_b v_a} \int_0^\infty du \left\{ \text{Re} \psi \left(1 + i \frac{\eta_{ab}}{u} \right) - \ln \frac{\eta_{ab}}{u} \right\} \left[\exp \left\{ -\frac{1}{2} \beta_b m_b v_a^2 (u-1)^2 \right\} - \exp \left\{ -\frac{1}{2} \beta_b m_b v_a^2 (u+1)^2 \right\} \right]. \quad (1.4)$$

The regular form is BPS (9.7); the singular form is BPS (9.5); the quantum form is BPS (10.27), where

$$\eta_{ab} = \frac{e_a e_b}{4\pi \hbar v_a}. \quad (1.5)$$

The Debye wavenumber K is arbitrary and will typically be chosen as $K = \kappa_e$. The function $F(v)$ takes the form

$$F(v) = - \int_{-\infty}^{\infty} du \frac{\rho_{\text{tot}}(u)}{v - u + i\eta} \quad \text{with} \quad \rho_{\text{tot}}(u) = \sum_b \rho_b(u) \quad (1.6)$$

$$\rho_b(v) = \kappa_b^2 \sqrt{\frac{\beta_b m_b}{2\pi}} v \exp \left\{ -\frac{1}{2} \beta_b m_b v^2 \right\}, \quad (1.7)$$

and its relation to the dielectric function is

$$k^2 \epsilon(\mathbf{k}, \mathbf{k} \cdot \mathbf{v}) = k^2 + F(\hat{\mathbf{k}} \cdot \mathbf{v}). \quad (1.8)$$

¹ By convention $b = 1$ will be the electron component.

The first term $C_{ab,R}^{\ell\ell<}$ arises from long-distance collective effects from the dielectric function, and it involves *all* plasma species (even species c different from a and b). This is the term I call non-separable, meaning that it cannot be written as a sum of individual plasma components involving only a single species. The second term $C_{ab,S}^{\ell\ell^c}$ arises from short-distance two-body classical scattering, and the third term $C_{ab}^{\ell\ell^{QM}}$ is the two-body quantum scattering correction to all orders in the quantum parameters $\bar{\eta}_{ab}$. Three body and higher effects are contained in our systematic error term, the next-to-next-to-leading order term proportional to g^3 . In a strongly coupled plasma these higher order effects dominate, but in a weakly coupled plasma they are negligible.

II. THE MAIN DRIVER

I will return the C -coefficients in three forms:

- i. `bps_ccoeff_ab_mass`: For a given pair of indices p and b (the projectile p will often be denoted by species index a), this routine returns the individual component $C_{ab}^{\ell\ell}(E)$ for a given energy E . The quantum parameter η can be arbitrary. This routine is used to construct the entries in the next two subroutines.
- ii. `bps_ccoeff_ab_matrix`: Returns the complete matrix of coefficients $C_{ab}^{\ell\ell}(E)$.
- iii. `bps_ccoeff_ei_mass`: This routine returns the sum over the ions $C_{pi}^{\ell\ell} = \sum_i C_{pi}^{\ell\ell}$ for a given projectile p . It also returns the coulomb logarithm.

A. The Driver Routine: `bps_ccoeff_ab_mass`

This subroutine returns the matrix of values $C_{ab}^{\ell\ell}(E)$ for a given energy E . The driving routine that calls and assembles the singular, regular, and quantum pieces.

`ccoeff.f90:bps_ccoeff_ab_mass`

```
!*** still need to fix scaling/units ***
!
!%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
! main driver for C-coefficient for general quantum and electron-mass regimes
!%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
!
SUBROUTINE bps_ccoeff_ab_mass(nni, ep, mp, zp, ia, ib, betab, zb, mb, nb, &
    c_ab, c_ab_sing, c_ab_reg, c_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       !
INTEGER,          INTENT(IN)    :: ia       !
INTEGER,          INTENT(IN)    :: ib       !
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
                                           ! C-coeffs [MeV/mic]

REAL,             INTENT(OUT)    :: c_ab
REAL,             INTENT(OUT)    :: c_ab_sing
REAL,             INTENT(OUT)    :: c_ab_reg
REAL,             INTENT(OUT)    :: c_ab_qm

REAL,             DIMENSION(1:nni+1) :: mpb, mbpb, kb2, ab
REAL,             :: vp, zp2, k, k2, kd, kd2, a, b, eta
REAL,             :: cc_r, cc_s, cq, c1, c2, c3

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 C-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  = 0.5*betab*mb*vp*vp/CC2 ! [dimensionless]
      IF (zb(ib) .NE. 0.) THEN ! ab=(1/2) betab(ib)*mbc2(ib)*vp2/CC2
        a  =ab(ib)
        b  =-Log(2*betab(ib)*BEKEV*ABS(zp*zb(ib))*k*A0CM*mbpb(ib) )-2*GAMMA
        eta=ABS(zp*zb(ib))*2.1870E8/vp ! defined with projectile velocity vp
        c1=2*zp2*BEKEV*kb2(ib)*A0CM    ! [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)/
        C3=CC/(betab(ib)*vp)           ! 1/betab(ib)*vp note: dE_\per/dx = C/m*c^2
        c3=c3/1000.                    ! convert from KeV to MeV
!
! C_{ab}-classical-singular
!
      CALL c_sing_mass(a,b,cc_s)
      c_ab_sing=c1*c2*c3*cc_s
!
! C_{ab}-classical-regular
!
      CALL c_reg_mass(nni,ia,ib,vp,k2,kb2,betab,mb,cc_r)
      c_ab_reg=c1*c3*cc_r
!
! C_{ab}-quantum
!
      CALL c_quantum_mass(ia,ib,a,eta,cq) ! eta = dimensionless quantum param.
      c_ab_qm=c1*c2*c3*cq
!
! C_{ab}-total
!
      c_ab=c_ab_sing + c_ab_reg + c_ab_qm
      ENDIF
      END SUBROUTINE bps_ccoeff_ab_mass

```

ccoeff.f90:bps_ccoeff_ab_matrix

```

!
! %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
! Assembles the matrix C_{ab} of the C-coefficients.
! %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
!
      SUBROUTINE bps_ccoeff_ab_matrix(nni, ep, betab, zb, mb, nb,      &
        c_ab, c_ab_sing, c_ab_reg, c_ab_qm, c_tot, c_i, c_e, cc_tot, &
        cc_i, cc_e, cq_tot, cq_i, cq_e, cc_s_i, cc_s_e, cc_r_i, cc_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,              INTENT(IN) :: zb       ! temp array [1/ke
      REAL,              INTENT(IN) :: mb       ! charge array
      REAL,              INTENT(IN) :: nb       ! mass array [keV]
      REAL,              INTENT(IN) ::          ! density [1/cc]
      REAL,              INTENT(IN) ::          ! C-coeffs [MeV/mic

```

```
REAL,      DIMENSION(1:nni+1,1:nni+1),INTENT(OUT) :: c_ab
REAL,      DIMENSION(1:nni+1,1:nni+1),INTENT(OUT) :: c_ab_sing
REAL,      DIMENSION(1:nni+1,1:nni+1),INTENT(OUT) :: c_ab_reg
REAL,      DIMENSION(1:nni+1,1:nni+1),INTENT(OUT) :: c_ab_qm
REAL,      DIMENSION(1:nni+1),          INTENT(OUT) :: c_tot
REAL,      DIMENSION(1:nni+1),          INTENT(OUT) :: c_i
REAL,      DIMENSION(1:nni+1),          INTENT(OUT) :: c_e
REAL,      DIMENSION(1:nni+1),          INTENT(OUT) :: cc_tot
REAL,      DIMENSION(1:nni+1),          INTENT(OUT) :: cc_i
REAL,      DIMENSION(1:nni+1),          INTENT(OUT) :: cc_e
REAL,      DIMENSION(1:nni+1),          INTENT(OUT) :: cq_tot
REAL,      DIMENSION(1:nni+1),          INTENT(OUT) :: cq_i
REAL,      DIMENSION(1:nni+1),          INTENT(OUT) :: cq_e
REAL,      DIMENSION(1:nni+1),          INTENT(OUT) :: cc_s_i
REAL,      DIMENSION(1:nni+1),          INTENT(OUT) :: cc_s_e
REAL,      DIMENSION(1:nni+1),          INTENT(OUT) :: cc_r_i
REAL,      DIMENSION(1:nni+1),          INTENT(OUT) :: cc_r_e

REAL      :: cab, cab_sing, cab_reg, cab_qm
REAL      :: mp, zp
INTEGER   :: ia, ib

c_i      = 0
cc_s_i   = 0
cc_r_i   = 0
cc_i     = 0
cq_i     = 0
DO ia=1,nni+1
  mp=mb(ia)
  zp=zb(ia)
  DO ib=1,nni+1
    CALL bps_ccoeff_ab_mass(nni, ep, mp, zp, ia, ib, betab, zb, mb, nb, &
      cab, cab_sing, cab_reg, cab_qm) !*! change to bps_acoeff_ab_mass
    c_ab(ia,ib) = cab
    c_ab_sing(ia,ib)=cab_sing
    c_ab_reg(ia,ib) =cab_reg
    c_ab_qm(ia,ib) =cab_qm
    IF (ib == 1) THEN
      c_e(ia) = cab
      cc_s_e(ia)= cab_sing
      cc_r_e(ia)= cab_reg
      cc_e(ia) = cab_sing + cab_reg
      cq_e(ia) = cab_qm
    ELSE
      c_i(ia) = c_i(ia) + cab
      cc_s_i(ia)= cc_s_i(ia) + cab_sing
      cc_r_i(ia)= cc_r_i(ia) + cab_reg
      cc_i(ia) = cc_i(ia) + cab_sing + cab_reg
      cq_i(ia) = cq_i(ia) + cab_qm
    ENDIF
  ENDDO
  c_tot(ia) = c_e(ia) + c_i(ia)
  cc_tot(ia)= cc_e(ia) + cc_i(ia)
  cq_tot(ia)= cq_e(ia) + cq_i(ia)
ENDDO
END SUBROUTINE bps_ccoeff_ab_matrix
```

ccoeff.f90:bps_ccoeff_ei_mass

```

!
!%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
! Returns C_{p I} = \sum_i C_{p i} for backward compatibility
!%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
!
SUBROUTINE bps_ccoeff_ei_mass(nni, ep, zp, mp, betab, zb, mb, nb, &
    c_tot, c_i, c_e, cc_tot, cc_i, cc_e, cq_tot, cq_i, cq_e, &
    cc_s_i, cc_s_e, cc_r_i, cc_r_e)
USE physvars
USE mathvars
USE controlvars
IMPLICIT NONE
INTEGER,          INTENT(IN)  :: nni      ! Plasma:
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
REAL,          INTENT(IN)  :: mp      ! projectile energy [keV]
REAL,          INTENT(IN)  :: zp      ! projectile mass [keV]
REAL,          INTENT(IN)  :: zp      ! projectile charge
!
REAL,          INTENT(OUT) :: c_tot   ! C-coeffs [MeV/micron]
REAL,          INTENT(OUT) :: c_i     ! electron + ion
REAL,          INTENT(OUT) :: c_e     ! ion contribution
REAL,          INTENT(OUT) :: cc_tot  ! electron contribution
REAL,          INTENT(OUT) :: cc_i    ! classical
REAL,          INTENT(OUT) :: cc_e    ! classical
REAL,          INTENT(OUT) :: cq_tot  ! quantum
REAL,          INTENT(OUT) :: cq_i    ! quantum
REAL,          INTENT(OUT) :: cq_e    ! quantum
REAL,          INTENT(OUT) :: cc_s_i
REAL,          INTENT(OUT) :: cc_s_e
REAL,          INTENT(OUT) :: cc_r_i
REAL,          INTENT(OUT) :: cc_r_e

REAL      :: cdum, cc_s, cc_r, cq
INTEGER   :: ia, ib, nnb

! initialize components of C-coefficients
!
c_tot = 0 ! electron + ion
c_i   = 0 ! ion contribution
c_e   = 0 ! electron contribution
cc_tot = 0 ! classical total
cc_e   = 0 ! classical electron
cc_i   = 0 ! classical ion
cq_tot = 0 ! quantum total
cq_e   = 0 ! quantum electron
cq_i   = 0 ! quantum ion
cc_s_i = 0
cc_s_e = 0
cc_r_i = 0
cc_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_ccoeff_ab_mass(nni, ep, mp, zp, ia, ib, betab, zb, mb, nb, &
    cdum, cc_s, cc_r, cq)
CALL x_collect(ib, NNB, cc_s, cc_r, cq, &

```



```

      c_tot, c_i, c_e, cc_tot, cc_i, cc_e, cq_tot,  &
      cq_i, cq_e, cc_s_i, cc_s_e, cc_r_i, cc_r_e)
    ENDIF
  ENDDO
END SUBROUTINE bps_ccoeff_ei_mass

```

B. The Regular Contribution: c_reg_mass

The long-distance regular contribution can be expressed as

$$C_{ab,R}^{\ell\ell<} = \frac{e_a^2}{4\pi} \frac{1}{\beta_b v_a} \frac{i}{2\pi} \int_{-1}^1 \frac{du}{u} \frac{\rho_b(v_a u)}{\rho_{\text{total}}(v_a u)} F(v_a u) \ln \left\{ \frac{F(v_a u)}{K^2} \right\} \quad (2.1)$$

$$= \frac{e_a^2}{4\pi} \frac{1}{\beta_b v_a} \frac{i}{2\pi} \int_0^1 \frac{du}{u} \frac{\rho_b(v_a u)}{\rho_{\text{total}}(v_a u)} \left[F(v_a u) \ln \left\{ \frac{F(v_a u)}{K^2} \right\} - F^*(v_a u) \ln \left\{ \frac{F^*(v_a u)}{K^2} \right\} \right] \quad (2.2)$$

$$= -\frac{e_a^2}{4\pi} \frac{1}{\beta_b v_a} \frac{1}{2\pi} \int_0^1 \frac{du}{u} \frac{\rho_b(v_a u)}{\rho_{\text{total}}(v_a u)} H(v_a u) , \quad (2.3)$$

where we have defined

$$H(v) \equiv -i \left[F(v) \ln \left\{ \frac{F(v)}{K^2} \right\} - F^*(v) \ln \left\{ \frac{F^*(v)}{K^2} \right\} \right] = 2 \left[F_{\text{Re}} \arg\{F\} + F_{\text{Im}} \ln \left\{ \frac{|F|}{K^2} \right\} \right] . \quad (2.4)$$

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

$$F(v) = K^2 \mathbb{F}(v) \quad \text{and} \quad H(v) = K^2 \mathbb{H}(v) . \quad (2.5)$$

Defining the parameters

$$a_c \equiv \left(\frac{\beta_c m_c}{2} \right)^{1/2} \quad (2.6)$$

$$\bar{\kappa}_c^2 \equiv \frac{\kappa_c^2}{K^2} \quad (2.7)$$

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

$$\mathbb{F}_{\text{Re}}(\{a_c v\}, \{\bar{\kappa}_c\}) = \sum_c \bar{\kappa}_c^2 \left(1 - 2a_c v \operatorname{daw}\{a_c v\} \right) \quad (2.8)$$

$$\mathbb{F}_{\text{Im}}(\{a_c v\}, \{\bar{\kappa}_c\}) = \sqrt{\pi} \sum_c \bar{\kappa}_c^2 a_c v e^{-a_c^2 v^2} . \quad (2.9)$$

The ratio of weighting factors can be written in terms of a function \mathbb{R}_{ab} defined by

$$\frac{\rho_b(v_a u)}{\rho_{\text{total}}(v_a u)} \cdot H(v_a u) = K^2 \frac{\rho_b(v_a u)}{\rho_{\text{total}}(v_a u)} \cdot \mathbb{H}(v_a u) \quad (2.10)$$

$$= K^2 \frac{\kappa_b^2 (\beta_b m_b / 2\pi)^{1/2} v_a u e^{-\frac{1}{2} \beta_b m_b v_a^2 u^2}}{\sum_c \kappa_c^2 (\beta_c m_c / 2\pi)^{1/2} v_a u e^{-\frac{1}{2} \beta_c m_c v_a^2 u^2}} \cdot \mathbb{H}(v_a u) \quad (2.11)$$

$$= \kappa_b^2 \cdot \underbrace{\left[\sum_c \frac{\kappa_c^2}{K^2} \left(\frac{\beta_c m_c}{\beta_b m_b} \right)^{1/2} e^{\frac{1}{2} (\beta_b m_b - \beta_c m_c) v_a^2 u^2} \right]^{-1}}_{\mathbb{R}_{ab}(v_a u)} \cdot \mathbb{H}(v_a u) \quad (2.12)$$

$$= \kappa_b^2 \mathbb{R}_{ab}(v_a u) \mathbb{H}(v_a u) . \quad (2.13)$$

We can now express the regular piece as

$$C_{ab,R}^{\ell\ell C} = \underbrace{\left[\frac{e_a^2 \kappa_b^2}{4\pi} \right]}_{c_{ab,1}} \cdot \frac{1}{\beta_b v_a} \cdot C_{ab,R}(v_a, \{a_c\}, \{\bar{\kappa}_c\}) \quad (2.14)$$

$$C_{ab,R}(v_a, \{a_c\}, \{\bar{\kappa}_c\}) = - \int_0^1 \frac{du}{u} \underbrace{\mathbb{R}_{ab}(\{a_c v_a u\}) \mathbb{H}(\{a_c v_a u\}, \{\bar{\kappa}_c\})}_{\text{d.cab_reg}} . \quad (2.15)$$

ccoeff.f90: d_cab_reg

```
!
!%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
! regular contribution for non-zero electron mass
!%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
!
SUBROUTINE c_reg_mass(nni, ia, ib, vp, k2, kb2, betab, mb, cc_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,             INTENT(IN)  :: betab
REAL,             INTENT(IN)  :: mb
REAL,             INTENT(OUT) :: cc_r
REAL,             DIMENSION(1:nni+1) :: ab
!
INTEGER, PARAMETER :: NR=10 ! integration regions: must be even
INTEGER, PARAMETER :: NR=100 ! integration regions: must be even
REAL,    PARAMETER :: UPM=0.7745966692E0 ! parameters for Gaussian Quad
REAL,    PARAMETER :: W13=0.5555555556E0, W2=0.8888888889E0
REAL      :: u0, u1, du, u, um, d_cab_reg
INTEGER    :: iu
ab=SQRT(0.5*betab*mb)*vp/CC
cc_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
```

```

      cc_r=cc_r+W2*d_cab_reg(u,vp,ia,ib,nni,k2,kb2,betab,mb)
      um=u-du*UPM
      cc_r=cc_r+W13*d_cab_reg(um,vp,ia,ib,nni,k2,kb2,betab,mb)
      um=u+du*UPM
      cc_r=cc_r+W13*d_cab_reg(um,vp,ia,ib,nni,k2,kb2,betab,mb)
    ENDDO
    cc_r=cc_r*du
  END SUBROUTINE c_reg_mass

  FUNCTION d_cab_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 ! Inv temperature array [1
  REAL,          DIMENSION(1:nni+1), INTENT(IN) :: mb ! Mass array [keV]
  REAL,          :: d_cab_reg! [dimensionless]
  REAL,          DIMENSION(1:nni+1) :: kbar2b, ab, ab2
  REAL,          :: fr, fi, fabs, farg, h, r_ib
  REAL,          :: kcb, bm_ic, bm_ib, a2_ic, a2_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))

  ! calculate spectral density
  r_ib=0
  bm_ib=betab(ib)*mb(ib)
  a2_ib =ab(ib)*ab(ib)
  DO ic=1,nni+1
    kcb=kb2(ic)/k2
    bm_ic=betab(ic)*mb(ic)
    a2_ic =ab(ic)*ab(ic)
    IF (ic == ib) THEN
      ex=1.
    ELSE
      au=(a2_ic-a2_ib)*u ! avoids exp of
      ex=EXP(-au)      ! large numbers
    ENDIF
    r_ib=r_ib + kcb*SQRT(bm_ic/bm_ib)*ex
  ENDDO
  r_ib=1./r_ib

  d_cab_reg=-r_ib*h/(u*TWOPI) ! See * in ccoeff_1.0.pdf
END FUNCTION d_cab_reg

```

C. The Singular Contribution: c_{sing}

The singular contribution,

$$C_{b,s}^{\ell c} = \left[\frac{e_p^2 \kappa_b^2}{4\pi} \left(\frac{\beta_b m_b}{2\pi} \right)^{1/2} v_p \right] \frac{1}{\beta_b v_p} \int_0^1 du u^{-1/2} e^{-\frac{1}{2} \beta_b m_b v_p^2 u} \left[-\ln \left\{ \frac{\beta_b e_b e_p}{4\pi} K \frac{m_b}{m_{pb}} \frac{u}{1-u} \right\} - 2\gamma \right], \quad (2.16)$$

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

$$\int_0^1 du u^{-1/2} e^{-\frac{1}{2} \beta_b m_b v_p^2 u} \left[\ln \left\{ \frac{u}{1-u} \right\} - \ln \left\{ \frac{\beta_b e_b e_p}{4\pi} K \frac{m_b}{m_{pb}} \right\} - 2\gamma \right], \quad (2.17)$$

which motivates the definition

$$C_{b,s}^{\ell\ell c} = c_{b,1} c_{b,2} c_{b,3} \cdot C_s(a_{pb}, b_{pb}) \quad (2.18)$$

$$C_s(a, b) = \int_0^1 du u^{-1/2} e^{-a u} \left[-\ln \left\{ \frac{u}{1-u} \right\} + b \right] \quad (2.19)$$

$$a_{pb} = \frac{1}{2} \beta_b m_b v_p^2 \quad \text{and} \quad b_{pb} = -\ln \left\{ \frac{\beta_b e_b e_p}{4\pi} K \frac{m_b}{m_{pb}} \right\} - 2\gamma \quad (2.20)$$

$$c_{b,1} = \frac{e_p^2 \kappa_b^2}{4\pi} \quad c_{b,2} = \left(\frac{\beta_b m_b v_p^2}{2\pi} \right)^{1/2} \quad c_{b,3} = \frac{1}{\beta_b v_p} \quad (2.21)$$

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

acoeff.f90: sing

```
!
! %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
! singular contribution for non-zero electron mass
! %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
!
SUBROUTINE c_sing_mass(a, b, cc_s)
  REAL,    INTENT(IN)    :: a
  REAL,    INTENT(IN)    :: b
  REAL,    INTENT(OUT)   :: cc_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
  cc_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
    cc_s=cc_s+W2*dcab_sing(u,a,b)
    um=u-du*UPM
    cc_s=cc_s+W13*dcab_sing(um,a,b)
    um=u+du*UPM
    cc_s=cc_s+W13*dcab_sing(um,a,b)
  ENDDO
  cc_s=cc_s*du
END SUBROUTINE c_sing_mass

!
! a = betab * mb * vp^2/ 2
!
FUNCTION dcab_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      :: dcab_sing ! [dimensionless]
  dcab_sing=EXP(-a*u)*(-LOG(u/(1-u)) + b)/SQRT(u) ! Eq BPS (9.5)
END FUNCTION dcab_sing
```

D. The Quantum Correction: c_quantum

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

$$C_b^{\ell\ell\text{QM}} = -\frac{e_p^2 \kappa_b^2}{4\pi} \left(\frac{\beta_b m_b}{2\pi} \right)^{1/2} v_p \frac{1}{\beta_b v_p} \int_0^\infty du \left[\text{Re} \psi \left\{ 1 + i \frac{\eta_{pb}}{u} \right\} - \ln \left\{ \frac{\eta_{pb}}{u} \right\} \right] \left[e^{-\frac{1}{2} \beta_b m_b v_p^2 (u-1)^2} - e^{-\frac{1}{2} \beta_b m_b v_p^2 (u+1)^2} \right]. \quad (2.22)$$

The quantum function we need to code is therefore

$$C_b^{\ell\ell\text{QM}} = \underbrace{\left[\frac{e_p^2 \kappa_b^2}{4\pi} \left(\frac{\beta_b m_b}{2\pi} \right)^{1/2} v_p \frac{1}{\beta_b v_p} \right]}_{c_{b,1} \cdot c_{b,2} \cdot c_{b,3}} \cdot C_1^{\text{QM}}(a_{pb}, \tilde{\eta}_{pb}), \quad (2.23)$$

where the arguments of the function are defined by

$$a_{pb} = \frac{1}{2} \beta_b m_b v_p^2 \quad (2.24)$$

$$\begin{aligned} \eta_{pb} &= \frac{e_p e_b}{4\pi \hbar v_p} = |Z_p Z_b| \frac{e^2}{8\pi a_0} \frac{2a_0}{\hbar} \frac{1}{v_p} = |Z_p Z_b| \cdot 13.606 \text{ eV} \cdot \frac{2 \cdot 5.29 \times 10^{-9} \text{ cm}}{6.5821 \times 10^{-16} \text{ eV s}} \frac{1}{v_p} \\ &= 2.1870 \times 10^8 \frac{|Z_p Z_b|}{v_p \cdot (\text{cm/s})^{-1}}, \end{aligned} \quad (2.25)$$

and the function itself takes the form

$$C_1^{\text{QM}}(a, \eta) = - \int_0^\infty du \left[\text{Re} \psi \left\{ 1 + i \frac{\eta}{u} \right\} - \ln \left\{ \frac{\eta}{u} \right\} \right] \left[e^{-a(u-1)^2} - e^{-a(u+1)^2} \right]. \quad (2.26)$$

acoeff.f90: quantum

```
!
!%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
! quantum contribution for non-zero electron mass
!%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
!
SUBROUTINE c_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=0.55555555556E0, W2=0.88888888889E0
  REAL :: dcq
  INTEGER :: iu
  aq=0.
  u0=0.
  ! choose plot range of gaussian e^{-a^2}
  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
    ! gaussian quadrature
    du=(u1-u0)/NQ
    u=u0-du
    DO iu=1,NQ,2 ! Gaussian quadrature
      u=u+2.E0*du
      aq=aq+W2*dcq(u,a,eta)
      um=u-du*UPM
      aq=aq+W13*dcq(um,a,eta)
      um=u+du*UPM
      aq=aq+W13*dcq(um,a,eta)
    ENDDO
    aq=aq*du
  END SUBROUTINE c_quantum_mass

  FUNCTION dcq(u, a, eta)
  USE physvars
  IMPLICIT NONE
  REAL,                                INTENT(IN)  :: u          ! [dimensionless]
  REAL,                                INTENT(IN)  :: a          ! [dimensionless]
  REAL,                                INTENT(IN)  :: eta        ! [dimensionless]
  REAL,                                :: dcq        ! [dimensionless]
  REAL                                :: repsi, eu, ep, em, psilog, ch, sh, csh
  eu = eta/u
  psilog = repsi(eu) - LOG(eu)
  em = EXP(-a * (u - 1)**2)
  ep = EXP(-a * (u + 1)**2)
  csh = em - ep
  dcq = -psilog*csh
  END FUNCTION dcq
```

Appendix A: Calculating the Real and Imaginary Parts of F

We can write the dielectric function (1.6) as a sum over plasma components,

$$F(v) = \sum_b F_b(v) , \quad (\text{A1})$$

where we express the contribution from plasma species b as

$$F_b(v) = - \int_{-\infty}^{\infty} du \frac{\rho_b(v)}{v - u + i\eta} \quad (\text{A2})$$

$$\rho_b(v) = \kappa_b^2 \sqrt{\frac{\beta_b m_b}{2\pi}} v \exp\left\{-\frac{1}{2} \beta_b m_b v^2\right\} . \quad (\text{A3})$$

We will often decompose F into its contribution from electrons and ions and write

$$F(v) = F_e(v) + F_i(v) . \quad (\text{A4})$$

Note the reflection property

$$F_b(-v) = F_b^*(v) , \quad (\text{A5})$$

which means that the real part of $F_b(v)$ is even in v and the imaginary part is odd. For numerical work it is best to use the explicit real and imaginary parts of F , which can be written

$$F_{\text{Re}}(v) = \sum_b \kappa_b^2 \left[1 - 2 \sqrt{\frac{\beta_b m_b}{2}} v \operatorname{daw}\left\{\sqrt{\frac{\beta_b m_b}{2}} v\right\} \right] \quad (\text{A6})$$

$$F_{\text{Im}}(v) = \sqrt{\pi} \sum_b \kappa_b^2 \sqrt{\frac{\beta_b m_b}{2}} v \exp\left\{-\frac{\beta_b m_b}{2} v^2\right\} = \pi \rho_{\text{tot}}(v) , \quad (\text{A7})$$

where the Dawson integral is defined by

$$\operatorname{daw}(x) = \int_0^x dy e^{y^2 - x^2} = \frac{\sqrt{\pi}}{2} e^{-x^2} \operatorname{erfi}(x) . \quad (\text{A8})$$

The limits of small and large arguments of the Dawson function are

$$\operatorname{daw}(x) = x + \frac{2x^3}{3} + \frac{4x^5}{15} + \mathcal{O}(x^7) \quad (\text{A9})$$

$$\operatorname{daw}(x) = \frac{1}{2x} + \frac{1}{4x^3} + \frac{3}{8x^5} + \mathcal{O}(x^{-7}) . \quad (\text{A10})$$

The functions $F_b(v)$ have units of wave-number-squared $[1/L^2]$ and their argument v has units of velocity. We can express the functions $F_b(v)$ in terms of a single dimensionless function $\mathbb{F}(x)$ as follows:

$$F_b(v) = \kappa_b^2 \mathbb{F}\left(\sqrt{\frac{\beta_b m_b}{2}} v\right) \quad (\text{A11})$$

with

$$\mathbb{F}(x) = \int_{-\infty}^{\infty} dy \frac{\bar{\rho}(y)}{y - x - i\eta} \quad (\text{A12})$$

$$\bar{\rho}(y) = \frac{1}{\sqrt{\pi}} y e^{-y^2} . \quad (\text{A13})$$

Relation (A11) holds because $\rho_b(u) = \kappa_b^2 \bar{\rho}(y)$ for $u = (2/\beta_b m_b)^{1/2} y$. The reflection property (A5) becomes

$$\mathbb{F}(-x) = \mathbb{F}^*(x) , \quad (\text{A14})$$

which means that the real part is even in x and the imaginary part is odd,

$$\mathbb{F}_{\text{Re}}(-x) = \mathbb{F}_{\text{Re}}(x) \quad (\text{A15})$$

$$\mathbb{F}_{\text{Im}}(-x) = -\mathbb{F}_{\text{Im}}(x) . \quad (\text{A16})$$

As with expressions (A6) and (A7), the real and imaginary parts can be written

$$\mathbb{F}_{\text{Re}}(x) = 1 - 2x \operatorname{daw}(x) \quad (\text{A17})$$

$$\mathbb{F}_{\text{Im}}(x) = \pi \bar{\rho}(x) = \sqrt{\pi} x e^{-x^2} . \quad (\text{A18})$$

Let us now establish the forms (A6) and (A7) for the real and imaginary parts of $F(v)$. Starting with

$$\frac{1}{y - x - i\eta} = \text{P} \frac{1}{y - x} + i\pi \delta(y - x) , \quad (\text{A19})$$

the imaginary part becomes

$$\mathbb{F}_{\text{Im}}(x) = \int_{-\infty}^{\infty} dy \operatorname{Im} \frac{\bar{\rho}(y)}{y - x - i\eta} = \int_{-\infty}^{\infty} dy \bar{\rho}(y) \pi \delta(y - x) = \pi \bar{\rho}(x) . \quad (\text{A20})$$

The real part of the function must be evaluated by a principal part integral,

$$\mathbb{F}_{\text{Re}}(x) = \text{P} \int_{-\infty}^{\infty} dy \frac{\bar{\rho}(y)}{y - x} . \quad (\text{A21})$$

Let us add and subtract unity in the form

$$\int_{-\infty}^{\infty} \frac{dy}{y} \bar{\rho}(y) = 1 , \quad (\text{A22})$$

so that

$$\mathbb{F}_{\text{Re}}(x) = 1 + \text{P} \int_{-\infty}^{\infty} dy \left[\frac{\bar{\rho}(y)}{y - x} - \frac{\bar{\rho}(y)}{y} \right] \quad (\text{A23})$$

$$= 1 + \text{P} \int_{-\infty}^{\infty} dy \frac{x}{y(y - x)} \bar{\rho}(y) \quad (\text{A24})$$

$$= 1 + \frac{x}{\sqrt{\pi}} \text{P} \int_{-\infty}^{\infty} dy \frac{e^{-y^2}}{y - x} . \quad (\text{A25})$$

Making the change of variables $y' = y - x$ (and dropping the prime) we can write

$$\mathbb{F}_{\text{Re}}(x) = 1 + \frac{x}{\sqrt{\pi}} \mathbf{P} \int_{-\infty}^{\infty} \frac{dy}{y} e^{-(y+x)^2} \quad (\text{A26})$$

$$= 1 + \frac{x e^{-x^2}}{\sqrt{\pi}} \mathbf{P} \int_{-\infty}^{\infty} \frac{dy}{y} e^{-y^2-2xy} \quad (\text{A27})$$

$$= 1 + \frac{x e^{-x^2}}{\sqrt{\pi}} \lim_{\epsilon \rightarrow 0^+} \left[\int_{-\infty}^{-\epsilon} \frac{dy}{y} e^{-y^2-2xy} + \int_{\epsilon}^{\infty} \frac{dy}{y} e^{-y^2-2xy} \right]. \quad (\text{A28})$$

In the last expression we have used the definition of the principal part integration. Making a change of variables $y' = -y$ in the first integral in square brackets gives (and again dropping the prime)

$$\int_{-\infty}^{-\epsilon} \frac{dy}{y} e^{-y^2-2xy} = - \int_{\epsilon}^{\infty} \frac{dy}{y} e^{-y^2+2xy}, \quad (\text{A29})$$

and this allows us to write

$$\mathbb{F}_{\text{Re}}(x) = 1 - \frac{x e^{-x^2}}{\sqrt{\pi}} \lim_{\epsilon \rightarrow 0^+} \int_{\epsilon}^{\infty} \frac{dy}{y} e^{-y^2} \left[e^{2xy} - e^{-2xy} \right]. \quad (\text{A30})$$

The term in square braces is just $2 \sinh(2xy)$, which renders the factor $1/y$ harmless when the limit $\epsilon \rightarrow 0^+$ is taken,

$$\mathbb{F}_{\text{Re}}(x) = 1 - \frac{2x e^{-x^2}}{\sqrt{\pi}} \int_0^{\infty} dy e^{-y^2} \frac{\sinh 2xy}{y} = 1 - 2x \text{daw}(x). \quad (\text{A31})$$

The latter form hold because this is just another integral representation of the Dawson function,

$$\text{daw}(x) = \frac{e^{-x^2}}{\sqrt{\pi}} \int_0^{\infty} dy e^{-y^2} \frac{\sinh 2xy}{y}. \quad (\text{A32})$$

Compare this with

$$\text{daw}(x) = e^{-x^2} \int_0^x dy e^{y^2}. \quad (\text{A33})$$