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A-Coefficient in Clog

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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 A-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 A-coefficients take the form

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

with

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

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

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

and

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

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 $\mathcal{A}_{b,R}^<$ 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 $\mathcal{A}_{b,s}^c$ arises from short-distance two-body classical scattering, and the third term $\mathcal{A}_b^{\text{QM}}$ 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 \mathcal{A} -coefficients in three forms:

- i. `bps_acoeff_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 $\mathcal{A}_{ab}(E)$ 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_acoeff_ab_matrix`: Returns the complete matrix of coefficients $\mathcal{A}_{ab}(E)$.
- iii. `bps_acoeff_ei_mass`: This routine returns the sum over the ions $\mathcal{A}_{pi} = \sum_i \mathcal{A}_{pi}$ for a given projectile p . It also returns the coulomb logarithm.

A. The Driver Routine: `bps_acoeff_ab_mass`

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

`acoeff.f90:bps_acoeff_ab_mass`

```

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)  :: mp       ! mass [keV]
REAL,             INTENT(IN)  :: zp       ! charge
INTEGER,          INTENT(IN)  :: ia       !
INTEGER,          INTENT(IN)  :: ib       !
REAL,             DIMENSION(1:nni+1),    INTENT(IN)  :: betab ! temp array [1/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
                                           ! A-coeffs [MeV/mic

REAL,             INTENT(OUT) :: a_ab
REAL,             INTENT(OUT) :: a_ab_sing
REAL,             INTENT(OUT) :: a_ab_reg
REAL,             INTENT(OUT) :: a_ab_qm

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

REAL, PARAMETER   :: EPS_SMALL_E=2.E-4
REAL, PARAMETER   :: EPS_SMALL_E_SING=2.E-4
REAL, PARAMETER   :: EPS_SMALL_E_REG=2.E-4

! initialize components of A-coefficients
!
kb2=8*PI*AOCM*BEKEV*zp*zp*nb*betab
kd2 = SUM(kb2) ! [1/cm^2]
kd  = SQRT(kd2) ! [1/cm]
k2  = kb2(1) ! [1/cm^2]
k   = SQRT(k2) ! [1/cm] k = k_e

! Loop over charged plasma species

```

```

        mpb = mp*mb/(mp+mb)           ! [keV]
        mbpb= mb/mpb                 ! [dimensionless]
        vp =CC*SQRT(2*ep/mp)         ! [cm/s]
        zp2=zp**2                    ! [dimensionless]
                                     ! ab=(1/2) betab(ib)*mbc2(ib)*vp2/CC2
        ab =0.5*betab*mb*vp*vp/CC2   ! [dimensionless]
        IF (zb(ib) .NE. 0.) THEN
        a =ab(ib)
        b =-Log(2*betab(ib)*BEKEV*ABS(zp*zb(ib))*k*A0CM*mbpb(ib) )-2*GAMMA+2
        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)/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(ib,nni,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

acoeff.f90:bps_acoeff_ab_matrix

    SUBROUTINE bps_acoeff_ab_matrix(nni, ep, 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)  :: betab   ! energy input [keV]
    REAL,             INTENT(IN)  :: zb      ! temp array [1/keV]
    REAL,             INTENT(IN)  :: mb      ! charge array
    REAL,             INTENT(IN)  :: nb      ! mass array [keV]
    REAL,             INTENT(IN)  :: nb      ! density [1/cc]
                                     !
                                     ! A-coeffs [MeV/micron]
    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              :: aab, aab_sing, aab_reg, aab_qm, mp, zp
    INTEGER           :: ia, ib

! Loop over charged plasma species
!
    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
    ENDDO
  ENDDO
END SUBROUTINE bps_acoeff_ab_matrix

```

acoeff.f90:bps_acoeff_ei_mass

```

      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 ! 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(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
      REAL,          INTENT(OUT) :: ac_s_e
      REAL,          INTENT(OUT) :: ac_r_i
      REAL,          INTENT(OUT) :: ac_r_e

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

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

```

```

NNB = nni+1                ! number of ions + electrons
ia=1
DO ib=1,nni+1
  IF (zb(ib) .NE. 0.) THEN
    CALL bps_acoeff_ab_mass(nni, ep, mp, zp, ia, ib, betab, zb, mb, nb, &
      adum, ac_s, ac_r, aq)
    CALL x_collect(ib, NNB, ac_s, ac_r, aq,      &
      a_tot, a_i, a_e, ac_tot, ac_i, ac_e, aq_tot, &
      aq_i, aq_e, ac_s_i, ac_s_e, ac_r_i, ac_r_e)
  ENDIF
ENDDO
END SUBROUTINE bps_acoeff_ei_mass

```

B. The Regular Contribution: a_reg_mass

The long-distance regular contribution can be expressed as

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

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

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

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

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

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

acoeff.f90: dab_reg

```

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/
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) :: alfb, ab
REAL,          :: fr, fi, fabs, farg, h, uvp
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
uvp=u*vp
CALL frfi(u,nni,alfb,ab,fr,fi,fabs,farg)
h=2*(fr*farg + fi*LOG(fabs))*u
!
! construct spectral weight ratio Rb=rho_b/rho_tot
!
r_ib=0
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=-r_ib*h/TWOPI
  END FUNCTION dab_reg

```

The numerical integration is performed by Gaussian quadrature:

acoeff.f90:

```

SUBROUTINE a_reg_mass(ib, nni, vp, k2, kb2, betab, mb, ac_r)
  IMPLICIT NONE
  INTEGER,                                INTENT(IN)  :: ib
  INTEGER,                                INTENT(IN)  :: nni
  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
  INTEGER, PARAMETER :: NR=10 ! integration regions: must be even
  REAL,   PARAMETER :: UPM=0.7745966692E0 ! parameters for Gaussian Quad
  REAL,   PARAMETER :: W13=0.5555555556E0, W2=0.8888888889E0
  REAL :: u0, u1, du, u, um, dab_reg
  INTEGER :: iu
  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_mass

```

C. The Singular Contribution: a_{sing}

The singular contribution,

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

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

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

which motivates the definition

$$\mathcal{A}_{b,s}^c = c_{b,1} c_{b,2} \cdot A_s(a_{pb}, b_{pb}) \quad (2.18)$$

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

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

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

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=0.55555555556E0, W2=0.88888888889E0
  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
```

D. The Quantum Correction: a-quantum

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

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

The quantum function we need to code is therefore

$$\mathcal{A}_b^{\text{QM}} = \underbrace{\left[\frac{e_p^2 \kappa_b^2}{4\pi} \left(\frac{\beta_b m_b}{2\pi} \right)^{1/2} v_p \right]}_{c_{b,1} \cdot c_{b,2}} \cdot A_1^{\text{QM}}(a_{pb}, \tilde{\eta}_{pb}), \quad (2.23)$$

where the arguments of the function are defined by

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

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

and the function itself takes the form

$$\begin{aligned} A_1^{\text{QM}}(a, \eta) &= - \int_0^\infty du \left[\text{Re} \psi \left\{ 1 + i \frac{\eta}{u} \right\} - \ln \left\{ \frac{\eta}{u} \right\} \right] \\ &\quad \frac{1}{2a u} \left[\left(e^{-a(u-1)^2} + e^{-a(u+1)^2} \right) - \frac{e^{-a(u-1)^2} - e^{-a(u+1)^2}}{2a u} \right]. \end{aligned} \quad (2.26)$$

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=0.55555555556E0, W2=0.88888888889E0
  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 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

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