Appendix A

Homogeneous Sphere

The theory underlying this appendix is given in Chapter 4; some of the computational aspects of Mie theory are discussed in Section 4.8.

Perhaps the best known program for computing Mie scattering coefficients is that by Dave (1968)—it is certainly one of the earliest to have a wide distribution. We have profited greatly from this program, and we would be remiss if we did not acknowledge our indebtedness to Dave. The subroutine BHMIE described in this appendix is, however, sufficiently different that it should not be considered as merely a minor variant form. We have borrowed tricks from here and there as well as added a few of our own, all with the aim of writing a simple, efficient program, easy to understand and hence easy to modify.

One of the major departures from the Dave program is that in BHMIE convergence of series is not determined by iteration. With the wisdom of hindsight, iteration seems inefficient because there is little disagreement about the approximate number of terms required for convergence: slightly more than x terms are sufficient, where x is the size parameter. We have tried various criteria, based more or less on guessing. After BHMIE was written, however, an extensive study was published by Wiscombe (1979, 1980), and we have modified our programs in the light of his work. Thus, series in BHMIE are terminated after NSTOP terms, where NSTOP is the integer closest to

$$x + 4x^{1/3} + 2.$$

A similar criterion was used by Wiscombe, who was guided by a suggestion by Khare and extensive computations. This criterion can, of course, be changed. But lest the reader with a large computer budget be seduced by the idea that if a certain number of terms is good then even more are better, we must issue a warning. Computation of ψ_n by forward recurrence is unstable, and roundoff error will eventually become unacceptable. Provided that one does not generate more orders of ψ_n than are needed for reasonable convergence, and that ψ_n is a double-precision variable, problems are not likely to be encountered with a computer of moderate size. But an attempt to squeeze out a few more decimal places might lead to disaster: scattering coefficients of order appreciably greater than NSTOP might be computed inaccurately, and greatly so, even though they are not really needed.

$D_n(mx)$ in the coefficients (4.88) is computed by the downward recurrence relation (4.89) beginning with D_{NMX}. Provided that NMX is sufficiently greater than NSTOP and $|mx|$, logarithmic derivatives of order less than NSTOP are remarkably insensitive to the choice of D_{NMX}; this is a consequence of the stability of the downward recurrence scheme for ψ_n. For vastly different choices of D_{NMX}, and a range of arguments mx, computed values of $D_{\text{NMX}-5}$ were independent of D_{NMX}. Thus, NMX is taken to be Max(NSTOP,$|mx|$) + 15 in BHMIE, and recurrence is begun with $D_{\text{NMX}} = 0.0 + i0.0$.

Both ψ_n and ξ_n, where $\xi_n = \psi_n - i\chi_n$, satisfy

$$\psi_{n+1}(x) = \frac{2n+1}{x}\psi_n(x) - \psi_{n-1}(x),$$

and are computed by this upward recurrence relation in BHMIE beginning with

$$\psi_{-1}(x) = \cos x, \qquad \psi_0(x) = \sin x,$$
$$\chi_{-1}(x) = -\sin x, \qquad \chi_0(x) = \cos x.$$

ψ_n is a double-precision and χ_n a single-precision variable.

The angle-dependent functions π_n and τ_n are computed by the upward recurrence relations (4.47). They need be computed only for scattering angles between 0 and 90° because of the relations (4.48).

Tests of BHMIE We have tested BHMIE thoroughly, which gives credence to its impeccability but does not guarantee it. In particular, we have never encountered any appreciable differences between results from BHMIE and those from Dave's program DBMIE. Aside from comparing results from BHMIE with those tabulated elsewhere or computed by other subroutines, there are several independent checks on any scattering program:

Q_{ext} and Q_{sca} must not be negative, and Q_{ext} must be greater than Q_{sca} except for a nonabsorbing sphere, in which instance they are equal. For very large size parameters the extinction efficiency approaches the limit 2. This might seem to be a good test of a program for large x. Q_{ext} oscillates about 2, however, and one is never sure if a deviation from 2 is a natural oscillation or an indicator of incipient error. We have found that a much more sensitive test of a program for large x is the asymptotic expression (4.83) for the backscattering efficiency. This seems not to be widely recognized, and it is worth mentioning here because it can be used to test other programs.

As a check on the amplitude scattering matrix elements, we compute Q_{ext} in BHMIE from the optical theorem (4.76), whereas Q_{sca} is computed from the series (4.61). POL, the degree of polarization, must vanish for scattering angles of 0 and 180°, as must S_{34}. Also, the 4 × 4 scattering matrix elements must satisfy

$$\left(\frac{S_{12}}{S_{11}}\right)^2 + \left(\frac{S_{33}}{S_{11}}\right)^2 + \left(\frac{S_{34}}{S_{11}}\right)^2 = 1$$

for all scattering angles.

```
      PROGRAM CALLBH (INPUT=TTY,OUTPUT=TTY,TAPE5=TTY)
C       ********************************************************
C       CALLBH CALCULATES THE SIZE PARAMETER (X) AND RELATIVE
C       REFRACTIVE INDEX (REFREL) FOR A GIVEN SPHERE REFRACTIVE
C       INDEX, MEDIUM REFRACTIVE INDEX, RADIUS, AND FREE SPACE
C       WAVELENGTH. IT THEN CALLS BHMIE, THE SUBROUTINE THAT COMPUTES
C       AMPLITUDE SCATTERING MATRIX ELEMENTS AND EFFICIENCIES
C       ********************************************************
      COMPLEX REFREL,S1(200),S2(200)
      WRITE (5,11)
C       ******************************************************
C       REFMED = (REAL) REFRACTIVE INDEX OF SURROUNDING MEDIUM
C       ******************************************************
      REFMED=1.0
C       *********************************************
C       REFRACTIVE INDEX OF SPHERE = REFRE + I*REFIM
C       *********************************************
      REFRE=1.55
      REFIM=0.0
      REFREL=CMPLX(REFRE,REFIM)/REFMED
      WRITE (5,12) REFMED,REFRE,REFIM
C       ********************************
C       RADIUS (RAD) AND WAVELENGTH (WAVEL) SAME UNITS
C       ********************************
      RAD=.525
      WAVEL=.6328
      X=2.*3.14159265*RAD*REFMED/WAVEL
      WRITE (5,13) RAD,WAVEL
      WRITE (5,14) X
C       ************************************************
C       NANG = NUMBER OF ANGLES BETWEEN 0 AND 90 DEGREES
C       MATRIX ELEMENTS CALCULATED AT 2*NANG - 1 ANGLES
C       INCLUDING 0, 90, AND 180 DEGREES
C       ************************************************
      NANG=11
      DANG=1.570796327/FLOAT(NANG-1)
      CALL BHMIE(X,REFREL,NANG,S1,S2,QEXT,QSCA,QBACK)
      WRITE (5,65) QSCA,QEXT,QBACK
      WRITE (5,17)
C       *************************************************
C       S33 AND S34 MATRIX ELEMENTS NORMALIZED BY S11.
C       S11 IS NORMALIZED TO 1.0 IN THE FORWARD DIRECTION
C       POL=DEGREE OF POLARIZATION (INCIDENT UNPOLARIZED LIGHT)
C       *************************************************
      S11NOR=0.5*(CABS(S2(1))**2+CABS(S1(1))**2)
      NAN=2*NANG-1
      DO 355 J=1,NAN
      AJ=J
      S11=0.5*CABS(S2(J))*CABS(S2(J))
      S11=S11+0.5*CABS(S1(J))*CABS(S1(J))
      S12=0.5*CABS(S2(J))*CABS(S2(J))
      S12=S12-0.5*CABS(S1(J))*CABS(S1(J))
      POL=-S12/S11
      S33=REAL(S2(J)*CONJG(S1(J)))
      S33=S33/S11
      S34=AIMAG(S2(J)*CONJG(S1(J)))
      S34=S34/S11
      S11=S11/S11NOR
      ANG=DANG*(AJ-1.)*57.2958
  355 WRITE (5,75) ANG,S11,POL,S33,S34
```

```
   65 FORMAT (//,1X,"QSCA= ",E13.6,3X,"QEXT = ",E13.6,3X,
     2"QBACK = ",E13.6)
   75 FORMAT (1X,F6.2,2X,E13.6,2X,E13.6,2X,E13.6,2X,E13.6)
   11 FORMAT (/"SPHERE SCATTERING PROGRAM"//)
   12 FORMAT(5X,"REFMED = ",F8.4,3X,"REFRE =",E14.6,3X,
     3"REFIM = ",E14.6)
   13 FORMAT (5X,"SPHERE RADIUS = ",F7.3,3X,"WAVELENGTH = ", F7.4)
   14 FORMAT (5X,"SIZE PARAMETER =",F8.3/)
   17 FORMAT(//,2X,"ANGLE",7X,"S11",13X,"POL",13X,"S33",13X,"S34"//)
      STOP
      END
C        ***********************************************************
C        SUBROUTINE BHMIE CALCULATES AMPLITUDE SCATTERING MATRIX
C        ELEMENTS AND EFFICIENCIES FOR EXTINCTION, TOTAL SCATTERING
C        AND BACKSCATTERING FOR A GIVEN SIZE PARAMETER AND
C        RELATIVE REFRACTIVE INDEX
C        ***********************************************************
      SUBROUTINE BHMIE (X,REFREL,NANG,S1,S2,QEXT,QSCA,QBACK)
      DIMENSION AMU(100),THETA(100),PI(100),TAU(100),PI0(100),PI1(100)
      COMPLEX D(3000),Y,REFREL,XI,XI0,XI1,AN,BN,S1(200),S2(200)
      DOUBLE PRECISION PSI0,PSI1,PSI,DN,DX
      DX=X
      Y=X*REFREL
C        ***********************************
C        SERIES TERMINATED AFTER NSTOP TERMS
C        ***********************************
      XSTOP=X+4.*X**.3333+2.0
      NSTOP=XSTOP
      YMOD=CABS(Y)
      NMX=AMAX1(XSTOP,YMOD)+15
      DANG=1.570796327/FLOAT(NANG-1)
      DO 555 J=1,NANG
      THETA(J)=(FLOAT(J)-1.)*DANG
  555 AMU(J)=COS(THETA(J))
C        *************************************************
C        LOGARITHMIC DERIVATIVE D(J) CALCULATED BY DOWNWARD
C        RECURRENCE BEGINNING WITH INITIAL VALUE 0.0 + I*0.0
C        AT J = NMX
C        *************************************************
      D(NMX)=CMPLX(0.0,0.0)
      NN=NMX-1
      DO 120 N=1,NN
      RN=NMX-N+1
  120 D(NMX-N)=(RN/Y)-(1./(D(NMX-N+1)+RN/Y))
      DO 666 J=1,NANG
      PI0(J)=0.0
  666 PI1(J)=1.0
      NN=2*NANG-1
      DO 777 J=1,NN
      S1(J)=CMPLX(0.0,0.0)
  777 S2(J)=CMPLX(0.0,0.0)
C        ***********************************************
C        RICCATI-BESSEL FUNCTIONS WITH REAL ARGUMENT X
C        CALCULATED BY UPWARD RECURRENCE
C        ***********************************************
      PSI0=DCOS(DX)
      PSI1=DSIN(DX)
      CHI0=-SIN(X)
      CHI1=COS(X)
      APSI0=PSI0
```

```
      APSI1=PSI1
      XI0=CMPLX(APSI0,-CHI0)
      XI1=CMPLX(APSI1,-CHI1)
      QSCA=0.0
      N=1
  200 DN=N
      RN=N
      FN=(2.*RN+1.)/(RN*(RN+1.))
      PSI=(2.*DN-1.)*PSI1/DX-PSI0
      APSI=PSI
      CHI=(2.*RN-1.)*CHI1/X - CHI0
      XI=CMPLX(APSI,-CHI)
      AN=(D(N)/REFREL+RN/X)*APSI - APSI1
      AN=AN/((D(N)/REFREL+RN/X)*XI-XI1)
      BN=(REFREL*D(N)+RN/X)*APSI - APSI1
      BN=BN/((REFREL*D(N)+RN/X)*XI - XI1)
      QSCA=QSCA+(2.*RN+1.)*(CABS(AN)*CABS(AN)+CABS(BN)*CABS(BN))
      DO 789 J=1,NANG
      JJ=2*NANG-J
      PI(J)=PI1(J)
      TAU(J)=RN*AMU(J)*PI(J) - (RN+1.)*PI0(J)
      P=(-1.)**(N-1)
      S1(J)=S1(J)+FN*(AN*PI(J)+BN*TAU(J))
      T=(-1.)**N
      S2(J)=S2(J)+FN*(AN*TAU(J)+BN*PI(J))
      IF(J.EQ.JJ) GO TO 789
      S1(JJ)=S1(JJ) + FN*(AN*PI(J)*P+BN*TAU(J)*T)
      S2(JJ)=S2(JJ)+FN*(AN*TAU(J)*T+BN*PI(J)*P)
  789 CONTINUE
      PSI0=PSI1
      PSI1=PSI
      APSI1=PSI1
      CHI0=CHI1
      CHI1=CHI
      XI1=CMPLX(APSI1,-CHI1)
      N=N+1
      RN=N
      DO 999 J=1,NANG
      PI1(J)=((2.*RN-1.)/(RN-1.))*AMU(J)*PI(J)
      PI1(J)=PI1(J)-RN*PI0(J)/(RN-1.)
  999 PI0(J)=PI(J)
      IF (N-1-NSTOP) 200,300,300
  300 QSCA=(2./(X*X))*QSCA
      QEXT=(4./(X*X))*REAL(S1(1))
      QBACK=(4./(X*X))*CABS(S1(2*NANG-1))*CABS(S1(2*NANG-1))
      RETURN
      END
```

SPHERE SCATTERING PROGRAM

REFMED = 1.0000 REFRE = .155000E+01 REFIM = 0.
SPHERE RADIUS = .525 WAVELENGTH = .6328
SIZE PARAMETER = 5.213

QSCA= .310543E+01 QEXT = .310543E+01 QBACK = .292534E+01

ANGLE	S11	POL	S33	S34
0.00	.100000E+01	0.	.100000E+01	0.
9.00	.785390E+00	-.459811E-02	.999400E+00	.343261E-01
18.00	.356897E+00	-.458541E-01	.986022E+00	.160184E+00
27.00	.766119E-01	-.364744E+00	.843603E+00	.394076E+00
36.00	.355355E-01	-.534997E+00	.686967E+00	-.491787E+00
45.00	.701845E-01	.959953E-02	.959825E+00	-.280434E+00
54.00	.574313E-01	.477927E-01	.985371E+00	.163584E+00
63.00	.219660E-01	-.440604E+00	.648043E+00	.621216E+00
72.00	.125959E-01	-.831996E+00	.203255E+00	-.516208E+00
81.00	.173750E-01	.341670E-01	.795354E+00	-.605182E+00
90.00	.124601E-01	.230462E+00	.937497E+00	.260742E+00
99.00	.679093E-02	-.713472E+00	-.717397E-02	.700647E+00
108.00	.954239E-02	-.756255E+00	-.394748E-01	-.653085E+00
117.00	.863419E-02	-.281215E+00	.536251E+00	-.795835E+00
126.00	.227421E-02	-.239612E+00	.967602E+00	.795798E-01
135.00	.543998E-02	-.850804E+00	.187531E+00	-.490882E+00
144.00	.160243E-01	-.706334E+00	.495254E+00	-.505781E+00
153.00	.188852E-01	-.891081E+00	.453277E+00	-.226817E-01
162.00	.195254E-01	-.783319E+00	-.391613E+00	.482752E+00
171.00	.301676E-01	-.196194E+00	-.962069E+00	.189556E+00
180.00	.383189E-01	0.	-.100000E+01	0.