```
' OPTIMIZATION  PROGRAM TO CALCULATE THE B GRADIENT BY VARYING emult (gamma)
' UNTIL ngraddiff  IS MINIMUM
' Dr Barry R. Clarke (aleteller@barryispuzzled.com)
' Completed 2 January 2024


' INSTRUCTIONS (30/12/25)
' (1) SET 'nn' range to first three states of the set
' (2) set 'emult' which is gamma in Eq. (13) hyperfine paper
' (3) Positive gamma is a different check to negative gamma
' (4) aim is to vary 'emult' until output 'ngraddiff' is minimized
' (5) at that point, read off 'B' from lower 'ngrad1'
' (6) These are logged in Tables (2) and (3) hyperfine paper

' ********************************************************************************


' CODATA (June 2019)
  alpha1 = 0.0072973525693    ' NIST: fine structure constant
  alpha2 = alpha1*alpha1      ' square of alpha1
  Rydfreq = 3289841960.2508   ' (MHz) NIST: Rydberg frequency, (1/2)*mo*alpha2*clight^2*10^(-6)/h
  Me = 9.1093837015*10^(-31)  ' (kg) NIST: electron rest mass
  clight = 299792458          ' (m/s), speed of light, CODATA (2018, 126)
  M = 0.000544617021488       ' NIST: e- to p+ rest mass ratio
  pi = 3.141592653589793
  h = 6.62607015*10^(-34)     '(J/Hz) Planck constant, CODATA (2018, 142)

' OUTPUT TEMPLATES
 template1$ = "###############.######"
 template2$ = "#####.##########"
 template3$ = "######.################"

 print ""

' NIST DATA: Hyperfine energy levels (MHz): Horbatsch and Hessels (2016, Tables 3 & 4)
xlogcoord = 0
ylogcoord = 0
xlogcoordstore = 0
ylogcoordstore = 0
xxlogcoordstore = 0
xylogcoordstore = 0

for nn = 1 to 3 ' set 1-6 for nS1/2, 7-12 for nP1/2, , 13-18 nP3/2, 19-24 for nD3/2, 25-30 for nD5/2
 select case
 case nn = 1
   print "1S1/2"
   NIST0 = 3288087922.4160      '1S(1/2) ionization energy (F=0)
   NIST1 = 3288086502.0102      '1S(1/2) ionization energy (F=1)
   n = 1
   L = 0
   Sp = 1/2
   case nn = 2
```

```
      print "2S1/2"
      NIST0 = 822025577.0922      '2S(1/2) (F=0)
      NIST1 = 822025399.5354      '2S(1/2) (F=1)
      n = 2
      L = 0
      Sp = 1/2

      case nn = 3
      print "3S1/2"
      NIST0 = 365343617.9043      '3S(1/2) (F=0)
      NIST1 = 365343565.2949      '3S(1/2) (F=1)
      n = 3
      L = 0
      Sp = 1/2

      case nn = 4
      print "4S1/2"
      NIST0 = 205505309.9525      '4S(1/2) (F=0)
      NIST1 = 205505287.7579      '4S(1/2) (F=1)
      n = 4
      L = 0
      Sp = 1/2

      case nn = 5
      print "5S1/2"
      NIST0 = 131523180.9882      '5S(1/2) (F=0)
      NIST1 = 131523169.6246      '5S(1/2) (F=1)
      n = 5
      L = 0
      Sp = 1/2

      case nn = 6
      print "6S1/2"
      NIST0 = 91335431.6017       '6S(1/2) (F=0)
      NIST1 = 91335425.0256       '6S(1/2) (F=1)
      n = 6
      L = 0
      Sp = 1/2
' ***************
     case nn = 7
      print "2P1/2"
      NIST0 = 822026546.1359      '2P(1/2) (F=0)
      NIST1 = 822026486.9664      '2P(1/2) (F=1)
      n = 2
      L = 1
      Sp = -1/2

      case nn = 8
      print "3P1/2"
      NIST0 = 365343906.4710      '3P(1/2) (F=0)
      NIST1 = 365343888.9392      '3P(1/2) (F=1)
      n = 3
```

```
      L = 1
      Sp = -1/2

      case nn = 9
      print "4P1/2"
      NIST0 = 205505431.9299      '4P(1/2) (F=0)
      NIST1 = 205505424.5337      '4P(1/2) (F=1)
      n = 4
      L = 1
      Sp = -1/2

      case nn = 10
      print "5P1/2"
      NIST0 = 131523243.5005      '5P(1/2) (F=0)
      NIST1 = 131523239.7136      '5P(1/2) (F=1)
      n = 5
      L = 1
      Sp = -1/2

      case nn = 11
      print "6P1/2"
      NIST0 = 91335467.7972       '6P(1/2) (F=0)
      NIST1 = 91335465.6058       '6P(1/2) (F=1)
      n = 6
      L = 1
      Sp = -1/2

      case nn = 12
      print "7P1/2"
      NIST0 = 67103543.4423       '7P1/2
      NIST1 = 67103542.0628
      n = 7
      L = 1
      Sp = -1/2

' ******************
     case nn = 13
       print "2P3/2"
      NIST0 = 822015547.4967      '2P(3/2) (F=1)
      NIST1 = 822015523.8451      '2P(3/2) (F=2)
      n = 2
      L = 1
      Sp = 1/2
      case nn = 14
      print "3P3/2"
      NIST0 = 365340647.6119      '3P(3/2) (F=1)
      NIST1 = 365340640.6040      '3P(3/2) (F=2)
      n = 3
      L = 1
      Sp = 1/2

      case nn = 15
```

```
    print "4P3/2"
    NIST0 = 205504057.1004      '4P(3/2) (F=1)
    NIST1 = 205504054.1439      '4P(3/2) (F=2)
    n = 4
    L = 1
    Sp = 1/2

    case nn = 16
    print "5P3/2"
    NIST0 = 131522539.5886      '5P(3/2) (F=1)
    NIST1 = 131522538.0749      '5P(3/2) (F=2)
    n = 5
    L = 1
    Sp = 1/2

    case nn = 17
    print "6P3/2"
    NIST0 = 91335060.4413       '6P(3/2) (F=1)
    NIST1 = 91335059.5653       '6P(3/2) (F=2)
    n = 6
    L = 1
    Sp = 1/2

    case nn = 18            ' Table IV
     print "7P3/2"
    NIST0 = 67103286.9157
    NIST1 = 67103286.3640
    n = 7
    L = 2
    Sp = -1/2

' ******************
    case nn = 19
    print "3D3/2"
    NIST0 = 365340651.1931      '3D(3/2) (F=1)
    NIST1 = 365340646.9865      '3D(3/2) (F=2)
    n = 3
    L = 2
    Sp = -1/2

    case nn = 20
    print "4D3/2"
    NIST0 = 205504058.6495      '4D(3/2) (F=1)
    NIST1 = 205504056.8748      '4D(3/2) (F=2)
    n = 4
    L = 2
    Sp = -1/2

    case nn = 21
    print "5D3/2"
    NIST0 = 131522540.3924      '5D(3/2) (F=1)
    NIST1 = 131522539.4837      '5D(3/2) (F=2)
```

```
    n = 5
    L = 2
    Sp = -1/2

    case nn = 22
    print "6D3/2"
    NIST0 = 91335060.9101       '6D(3/2) (F=1)
    NIST1 = 91335060.3843       '6D(3/2) (F=2)
    n = 6
    L = 2
    Sp = -1/2

   case nn = 23            ' Table V
     print "7D3/2"
    NIST0 = 67103287.2124
    NIST1 = 67103286.8813
    n = 7
    L = 2
    Sp = -1/2

    case nn = 24
     print "8D3/2"
    NIST0 = 51375939.6283
    NIST1 = 51375939.4065
    n = 8
    L = 2
    Sp = -1/2

' ***************
   case nn = 25
    print "3D5/2"
    NIST0 = 365339566.8037      '3D(5/2) (F=2)
    NIST1 = 365339564.1003      '3D(5/2) (F=3)
    n = 3
    L = 2
    Sp = 1/2
    case nn = 26
    print "4D5/2"
    NIST0 = 205503601.1722      '4D(5/2) (F=2)
    NIST1 = 205503600.0315      '4D(5/2) (F=3)
    n = 4
    L = 2
    Sp = 1/2
    case nn = 27
    print "5D5/2"
    NIST0 = 131522306.1639      '5D(5/2) (F=2)
    NIST1 = 131522305.5800      '5D(5/2) (F=3)
    n = 5
    L = 2
    Sp = 1/2
    case nn = 28
    print "6D5/2"
```

```
    NIST0 = 91334925.3612       '6D(5/2) (F=2)
    NIST1 = 91334925.0233       '6D(5/2) (F=3)
    n = 6
    L = 2
    Sp = 1/2
    case nn = 29                ' 7D5/2
    print "7D5/2"
    NIST0 = 67103201.8522
    NIST1 = 67103201.6394
    n = 7
    L = 2
    Sp = 1/2
    case nn = 30                ' 8D5/2
    print "8D5/2"
    NIST0 = 51375882.4437
    NIST1 = 51375882.3011
    n = 8
    L = 2
    Sp = 1/2
' ************ END
   case nn = 31
    print "1S1/2"
    NIST0 = 3288087922.4160       '1S(1/2) ionization energy (F=0)
    NIST1 = 3288086502.0102       '1S(1/2) ionization energy (F=1)
    n = 1
    L = 0
    Sp = 1/2
   case nn = 32
     print "2P3/2"
    NIST0 = 822015547.4967       '2P(3/2) (F=1)
    NIST1 = 822015523.8451       '2P(3/2) (F=2)
    n = 2
    L = 1
    Sp = 1/2
    case nn = 33
    print "3D5/2"
    NIST0 = 365339566.8037       '3D(5/2) (F=2)
    NIST1 = 365339564.1003       '3D(5/2) (F=3)
    n = 3
    L = 2
    Sp = 1/2
   case nn = 34            ' Table VI, Horbatsch (circle)
     print "4F7/2"
    NIST0 = 205503373.1403         ' 4F(7/2) (F=4)
    NIST1 = 205503372.5369         ' 4F(7/2) (F=5)
    n = 4
    L = 3
    Sp = 1/2
   case nn = 35            ' Table VI, Horbatsch (circle)
    print "5G9/2"
    NIST0 = 131522119.3650         ' 5G9/2
    NIST1 = 131522119.1739         '
```

```
    n = 5
    L = 4
    Sp = 1/2
   case nn = 36          ' Table VI, Horbatsch (circle)
    print "6H11/2"
    NIST0 = 91334790.2371       ' 6H11/2
    NIST1 = 91334790.1619       '
    n = 6
    L = 5
    Sp = 1/2
   case nn = 37          ' Table VI, Horbatsch (circle)
    print "7I13/2"
    NIST0 = 67103104.6046       ' 7I13/2
    NIST1 = 67103104.5703       '
    n = 7
    L = 6
    Sp = 1/2
    case nn = 38          ' Table VI, Horbatsch (circle)
    print "8K15/2"
    NIST0 = 51375811.1884       ' 8K15/2
    NIST1 = 51375811.1710       '
    n = 8
    L = 7
    Sp = 1/2
    case nn = 39          ' Table VI, Horbatsch (circle)
    print "9L17/2"
    NIST0 = 40593231.0941       ' 9L17/2
    NIST1 = 40593231.7483       '
    n = 9
    L = 8
    Sp = 1/2

  end select
  print " nn = ";nn


' SOMMERFELD/MVR FINE STRUCTURE QUANTUM NUMBERS
  na = L + Sp + 0.5       ' azimuthal quantum number
  nr = n - na             ' radial quantum number
  Y = nr + sqr(na*na - alpha2) ' Kalpha = 1
  Y2 = Y*Y

Xjump = 0
gosub [coordinates]   ' calculates r2f2 and gives coordinates to evel3
r2f2 = Xstore^2 + (1 - M)^2
krel = sqr(1 - alpha2/(2*(Y^2 + alpha2)))

' Select gamma in hyperfine paper Eq. (13)
emult = 1.006942700  ' nS1/2 B = -3.0000421859595
'emult = -0.549012    ' nS1/2 B = -2.999976494243
'emult = 0.55773890261   ' nP1/2 B = -3.00000946384
'emult = -0.20481644002   ' nP1/2 B = -3.000001596923
```

```
'emult = 0.48878536995    ' nP3/2 B = -3.00000976361
'emult = -0.23361014241    ' nP3/2 B = -3.000002303498
'emult = 0.3957755         ' nD3/2 B = -3.000004673972
'emult = -0.1836735         ' nD3/2 B = -3.000002402484
'emult = 0.37459705         ' nD5/2 B = -3.000004778242
'emult = -0.1950811          ' nD5/2 B = -3.0000023717

evel3 = (1 + emult*M/n)^2

 gosub [MVRfs2]

Xjump = 1
 gosub [coordinates]

 xlogcoord = log(sqr(r2f2))
 ylogcoord = log(abs(VortexEnergy2 - (NIST0 + NIST1)/2))

 if (nn > 1 and nn <= 6) or (nn > 7 and nn <= 12) or (nn > 13 and nn <= 18) or (nn > 19 and nn <= 24) or (nn >
25 and nn <= 30) or (nn > 31 and nn <= 39) then

   ngrad1 = (ylogcoord - ylogcoordstore)/(xlogcoord - xlogcoordstore)
  print "ngrad1     = ";using (template3$,ngrad1)
   ngraddiff =   ngradstore - ngrad1
  print "ngraddiff  = ";using (template3$,ngraddiff)
  ngradstore = ngrad1
  print ""
 end if

  xlogcoordstore = xlogcoord
  ylogcoordstore = ylogcoord

next nn

print " done"
  end


' MVR FINE STRUCTURE ENERGY

[MVRfs2]

  evel3aa = nr + sqr(na*na - alpha2*evel3)
  evel3bb = evel3aa*evel3aa
  evel3cc = alpha2*evel3/(evel3bb)
  evel3dd = evel3cc/(2*(1 + evel3cc))
  evel3ee = sqr(1 - evel3dd)
  evel3ff = evel3bb + alpha2*evel3
  k2 = M/evel3ee
  redmass3 = 1/(1 + k2)
  VortexEnergy2 = redmass3*evel3*Rydfreq/(evel3ee*evel3ff)
  print ""
```

```
return


' PROTON-ELECTRON SEPARATION (P.E. = K.E.)
[coordinates]
' CONDUCTED IN CENTER OF MASS FRAME SO NO evel3
' SEARCH ROUTINE TO LOCATE EMISSION X COORDINATE RELATIVE TO PROTON Sp-2 CENTRE
 Xinc = 0              ' initialize increment for X search
 Xstore = 0            ' initialize memorized value of X
 for acc = -1 to 14    ' variable controlling decimal place searched
 for msearch = 0 to 150 ' raised upper limit for high x, only 0-10 reqd for decimal places

  Xinc = msearch/10^(acc) ' increment added to previous trial X
  X = Xstore + Xinc      ' stores trial value of X coordinate, as fraction of ground state radius
  XX = X
  R1 = M
R2 = alpha1/sqr(1 - alpha2)

FX1 = 1  ' **** from (54)
FX2 = n*sqr(1 + alpha2/Y^2)*(1 - alpha2)
FX3 = FX1/FX2

  Fint1 = 1 - R1
  Fint2 = 1 + (XX*XX + R2*R2)/(Fint1*Fint1)
  Fint3 = 1/(Fint1*sqr(Fint2))
  Fint4 = R2*R2*(XX*XX + Fint1*Fint1)/(Fint1^4*Fint2^2)
  Fint5 = Fint4*Fint4
  Fint = Fint3*(1 + (3/4)*Fint4 + (105/64)*Fint5)
  FX = FX3*Fint

 Felectron = (0.5/(Y^2 + alpha2))*(1/sqr(1 - alpha2/(2*(Y^2 + alpha2))))
' Eq. (85) in Photonic toroidal vortex model paper
 Fsearch = FX - Felectron

  if Fsearch < 0 then  ' attach marker value to sign of Fsearch
   mark = 0
  else
   mark = 1
  end if

  if msearch > 0 then  ' only compare Fsearch sign with previous one only after first pass
   if mark <> storemark then
    Xstore = Xstore + (msearch - 1)/10^acc  ' return to previous digit in search
    msearch = 10
   end if
  end if

  storemark = mark  ' store present Fsearch sign

  next msearch
  next acc
```

```
 return


' *** END OF PROGRAM ***
```