# A PROGRAM TO COMPUTE EXACT HYDROGENIC OSCILLATOR STRENGTHS, EINSTEIN COEFFICIENTS, AND LIFETIMES

D. Hoang-Binh
LERMA, BAT 18, Observatoire de Paris-Meudon, F-92195 Meudon Principal Cedex, France

## Abstract

An exact expression for the dipole radial integral of hydrogen has been given by Gordon [Ann. Phys. 2 (1929) 1031]. It contains two hypergeometric functions $F(a,b;c;x)$, which are difficult to calculate directly, when the (negative) integers a, are large, as in the case of high Rydberg states of hydrogenic ions. We have derived a simple method [D. Hoang-Binh, Astron.Astrophys. 238 (1990) 449], using a recurrence relation to calculate exactly F, starting from two initial values, which are very easy to compute. We present here a numerical code using this method, to compute exact hydrogenic oscillator strengths, Einstein coefficients, and lifetimes.

## Program summary

Title of program: HEINF.f
Computers: all computers with a Fortran 77 compiler
Operating system used: MacOS 9.0
Programming language used: Fortran 77
Nature of physical problem: Exact calculation of atomic data.
Method of solution: Use of recursion relation.
Typical run time: 2s

## 1. Introduction

*The dipole moment corresponding to the transition from the upper state (n,l) to the lower state (n',l') of a hydrogenic ion of nuclear charge Z is (see e.g. [3])*

$$R(n,l;n',l') = \int P_{n,l}(r)\ r^3\ P_{n',l'}(r)\ dr,$$

*the integration range being (0,infinity),*

*where $P_{n,l}(r)$ and $P_{n',l'}(r)$ are the radial wave functions of the states (n,l) and (n',l'), respectively. Gordon [1] has derived an exact expression for this radial integral,*

$$R(n,l;n',l') = (-1)^{n'-1}[4(2l-1)!]^{-1}[(n+l)!$$
$$(n'+l-1)!/(n-l-1)!(n'-l)!]^{1/2}$$
$$x(4nn')^{l+1}\ (n-n')^{n+n'-2l-2}\ (n+n')^{-n-n'}$$
$$x\{F(-n+l+1,-n'+l;2l;-4nn'/[n-n']^2)$$
$$-(n-n')^2(n+n')^{-2}F(-n+l-1,-n'+l;2l;-4nn'/[n-n']^2)\}$$
<div align="right">(1)</div>

*However, it is rather difficult to calculate the hypergeometric function*

$$F(a,b;c;x) = 1 + [ab/c(1!)]X + [a(a+1)b(b+1)/c(c+1)(2!)]x^2 + \ldots$$

*when n and n' are large, as in the case of Rydberg states.*

*Many tables have been published. However, they are either limited to rather small values of n, n'[3–5], or restricted to values of total oscillator strengths, without partition with respect to the orbital quantum number [6]. They do not cover the whole range of dipole transitions encountered in physics and astronomy, where high Rydberg states with*

principal quantum numbers n>100 have become quite common.

Many authors (e.g., [7–10]) have proposed approximate expressions, valid only in limited ranges of n, n', l, l'. In this paper, we present a simple numerical code, based on an earlier theoretical paper [2], for calculating exactly the dipole integral, and consequently the related oscillator strengths, Einstein coefficients, and lifetimes. It is easy to programme, even with a pocket calculator, and works well for n and n' as high as 1000.

2. Outline of the method

Because a,b≤0, the two hypergeometric functions in (1) are in fact two polynomials, whose degrees may be very large, if n,n'>>1. We have found that, for many transitions, the direct calculation of F is problematic, as it requires a great number of significant digits.

We use a new procedure, described in previous papers [2,11], which allows an easy calculation of the Gordon formula for Rydberg states as high as 1000.

It is clear from (1) that the only difficulty in computing the radial integrals resides in the evaluation of the hypergeometric functions. Fortunately, use can be made of the following recurrence relation (see e.g. [12])

$$(a-c)F(a-1)=a(1-x)[F(a)-F(a+1)]+(a+bx-c)F(a), \quad (3)$$

where F(a)=F(a,b;c;x). The two adopted initial values are F(0)=1 and F(-1)=1-(b/c)x. After having calculated the functions F in (1), the values of the radial integral R(n,l;n',l') and the corresponding oscillator strength may be obtained without difficulty.

Since F(a,b;c;x)= F(b,a;c,x), the relation (3), hereafter referred to as 'a' recurrence, may also be

used for a recurrence on b. In fact, we have found that for large quantum numbers, 'b' recurrence is stable for l'=l-1, and 'a' recurrence is stable for l'=l++1, and the code has been constructed accordingly.

## 3. Practical procedure

3.1. Calculate the parameters of $F(a,b;c;x)$.
From (1),they are

$$a=-n+l+1; \quad b=-n'+l; \quad c=2l; \quad x=-4nn'/[n-n']^2$$

3.2. Calculate the two hypergeometric functions in (1), starting from

$$F(0)= F(0,b;c;x)=1; \quad F(-1)= F(-1,b;c;x)= 1-bx/c$$

to obtain, via (3) $F(-n+l\pm1)$.

3.3. Calculate the radial integral given by (1).

3.4. Calculate the absorption oscillator strength, given by

$$f(n,l;n',l')=(1/3)(u/Ry) \quad [max(l,l')/(2l'+1)] \; [R(n,l;n',l')]^2$$

where Ry is the Rydberg constant, in the same units as the frequency of the transition $(n,l) \rightarrow (n',l')$.

3.5. Calculate the Einstein transition probability, given by

$$A(n,l;n',l')=(64\pi^4 \upsilon^3/3hc^3)[max(l',l)/(2l+1)e^2 a_0^2 \; [R(n,l;n',l')]^2$$

where h=Planck constant, c=velocity of light, e=electron charge, and $a_0$=Bohr radius.

*3.6. Calculate the total Einstein coefficient, given by*

$$A(n,n') = \sum_{l,l'} (2l+1)/n^2 \, A(n,l;n',l'),$$

*from which the radiative lifetime T can be calculated;*

$$T_n = 1/\sum_{n'} A_{n,n'}$$

## 4. Results and discussion

*The method is very simple to programme, even with a pocket programmable calculator. We have thus been able to reproduce the tables published by [4], who considered mainly principal quantum numbers $n,n' \leq 20$. Values of $R(n,l;n',l')$ may be obtained for $n,n'$ as high as 1000, meeting amply the needs in studies of high Rydberg states. It is easier to handle than approximate expressions given by [8–10]. These have only limited ranges of validity; and involve Bessel functions [8,9] or McDonald functions [10], which, paradoxically, appear to be more difficult to calculate than the hypergeometric functions in our method.*

*Since good accuracy has been achieved with simple precision arithmetics, the change to a double precision version, though easy to perform, has not been considered necessary*

*Finally, it may be noted that quantum numbers close to 1000 are not sheer curiosity; they have been actually involved in radio recombination lines observed in interstellar CII–HI clouds.*

## 5. Program description

*Program HEINF.f calls the subroutines faz5 and fbz5, corresponding to the cases $l'=l+1$ and $l'=l-1$, respectively.*

*The input data is written on the file HEIN.in,*

*nu= upper state principal quantum number n,*
*nl= lower state principal quantum number n',*
*z= nuclear charge (z= 1 for hydrogen, 2 for He+,etc.),*
*am= nuclear mass M in atomic mass units.*

*The output data is written to unit 5 on the file ba5.out.*

*Each subroutine generates the absolute value of the dipole radial integral (ain=|R(n,l;n',l')|), its square (ain2=|R(n,l;n',l')|2), the absorption oscillator strength (os= f(n',l';n,l)), and the Einstein coefficient (ein= A(n,l;n',l')), for the transition (n,l)-(n',l'). The quantity*

$$einl = (2l+1)/n^2 \ A(n,l;n',l'),$$

*is also calculated, in order to get the total Einstein coefficient, A(n,n'), and the life time $T_n$ of level n.*

*Appendix A*

*A.1. Test run input*

*HEIN.in*
*0020 0011 +1.0E+00 +1.0E+00 nu nl z am*


*A.2. Test run output*

*HEIN.out*

Z= 1.0000E+00        M= 1.0000E+00
nu= 20   nl= 19

```
   lu      ll     R**2            f(nl,ll;nu,lu)    A(nu,lu;nl,ll)
```

| | | | | |
|---|---|---|---|---|
| 1 | 0 | 1.7474E+04 | 1.5732E+00 | 3.0693E+02 |
| 2 | 1 | 1.9958E+04 | 1.1978E+00 | 4.2066E+02 |
| 3 | 2 | 2.2715E+04 | 1.2270E+00 | 5.1296E+02 |
| 4 | 3 | 2.5772E+04 | 1.3258E+00 | 6.0357E+02 |
| 5 | 4 | 2.9161E+04 | 1.4585E+00 | 6.9845E+02 |
| 6 | 5 | 3.2912E+04 | 1.6162E+00 | 8.0041E+02 |
| 7 | 6 | 3.7062E+04 | 1.7966E+00 | 9.1135E+02 |
| 8 | 7 | 4.1647E+04 | 1.9997E+00 | 1.0327E+03 |
| 9 | 8 | 4.6715E+04 | 2.2265E+00 | 1.1660E+03 |
| 10 | 9 | 5.2311E+04 | 2.4787E+00 | 1.3126E+03 |
| 11 | 10 | 5.8488E+04 | 2.7581E+00 | 1.4740E+03 |
| 12 | 11 | 6.5303E+04 | 3.0673E+00 | 1.6517E+03 |
| 13 | 12 | 7.2820E+04 | 3.4090E+00 | 1.8475E+03 |
| 14 | 13 | 8.1106E+04 | 3.7861E+00 | 2.0632E+03 |
| 15 | 14 | 9.0236E+04 | 4.2019E+00 | 2.3007E+03 |
| 16 | 15 | 1.0030E+05 | 4.6605E+00 | 2.5625E+03 |
| 17 | 16 | 1.1139E+05 | 5.1659E+00 | 2.8508E+03 |
| 18 | 17 | 1.2360E+05 | 5.7227E+00 | 3.1685E+03 |
| 19 | 18 | 1.3705E+05 | 6.3358E+00 | 3.5182E+03 |
| | | | | |
| 0 | 1 | 1.3234E+04 | 3.9714E-01 | 6.9734E+02 |
| 1 | 2 | 1.1435E+04 | 4.1177E-01 | 4.0168E+02 |
| 2 | 3 | 9.8241E+03 | 3.7905E-01 | 3.1060E+02 |
| 3 | 4 | 8.3863E+03 | 3.3555E-01 | 2.5251E+02 |
| 4 | 5 | 7.1057E+03 | 2.9078E-01 | 2.0801E+02 |
| 5 | 6 | 5.9691E+03 | 2.4802E-01 | 1.7156E+02 |
| 6 | 7 | 4.9638E+03 | 2.0854E-01 | 1.4084E+02 |
| 7 | 8 | 4.0788E+03 | 1.7280E-01 | 1.1463E+02 |
| 8 | 9 | 3.3041E+03 | 1.4090E-01 | 9.2174E+01 |
| 9 | 10 | 2.6304E+03 | 1.1277E-01 | 7.2950E+01 |
| 10 | 11 | 2.0496E+03 | 8.8248E-02 | 5.6571E+01 |
| 11 | 12 | 1.5542E+03 | 6.7162E-02 | 4.2729E+01 |
| 12 | 13 | 1.1376E+03 | 4.9312E-02 | 3.1171E+01 |
| 13 | 14 | 7.9383E+02 | 3.4501E-02 | 2.1689E+01 |
| 14 | 15 | 5.1752E+02 | 2.2544E-02 | 1.4105E+01 |
| 15 | 16 | 3.0397E+02 | 1.3268E-02 | 8.2670E+00 |
| 16 | 17 | 1.4894E+02 | 6.5128E-03 | 4.0430E+00 |
| 17 | 18 | 4.8703E+01 | 2.1331E-03 | 1.3198E+00 |

nu= 20   nl= 19    A(nu,nl)= 2.0649E+03

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