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# An implementation of atomic form factors<sup>☆</sup>

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## Abstract

A FORTRAN implementation of hydrogen-like discrete–discrete atomic form factors is presented. The definition of atomic form factors and their applicability to the calculation of atomic cross sections is briefly discussed. An explicit analytical expression for the discrete–discrete atomic form factors is presented exactly in the way they are implemented in the program. Finally, a description of the program itself and how to use it is given, together with some useful examples and their outputs.

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Keywords: Atomic form factors; Atomic scattering; Cross sections

## PROGRAM SUMMARY

*Title of program:* DIFOFA

*Catalog identifier:* ADQY

*Program Summary URL:* <http://cpc.cs.qub.ac.uk/summaries/ADQY>

*Program obtainable from:* CPC Program Library, Queen's University of Belfast, N. Ireland; <http://www.usc.es/gaes/difofa.html>

*Operating systems under which the program has been tested:* The program has been successfully tested in a SUN workstation running on Solaris 2.6 and with several distributions of Linux (RedHat, Debian) running on different kernels (2.2.19, 2.4.7–10, etc.)

*Programming language used:* FORTRAN 77

*Memory required to execute with typical data:* size of each of the two test executable programs is approximately 120 kB

*No. of processors used:* 1

*Has the code been vectorized or parallelized?:* no

*No. of bytes in distributed program, including test data, etc.:* 6796

*Distribution format:* tar gzip file

*Keywords:* Atomic form factors, atomic scattering, cross sections

*Nature of physical problem*

The scattering of an electron or a proton by a hydrogen-like atom or the collision of a hydrogen-like atom with a more complex atom

<sup>☆</sup> This program can be downloaded from the CPC Program Library under catalogue identifier: <http://cpc.cs.qub.ac.uk/summaries/ADQY>

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are three body systems which can be solved perturbatively. The first order solution corresponds to a one photon exchange interaction and is known as the first Born approximation [1–3]. The response of the hydrogen-like atom to a definite momentum of the exchanged photon is given by the Fourier transform of its charge density, known as the atomic form factor. The hydrogen-like form factors have been studied in the framework of hydrogen–electron collisions and the recent experiments on exotic atoms [4,5] have updated the interest on this topic requiring the knowledge of the form factors of highly excited states.

#### Method of solution

We have considered an analytical expression of the hydrogen-like atomic form factors [7] and we have implemented it in a FORTRAN code optimizing the addition method and testing the final result.

## LONG WRITE-UP

### 1. Introduction

The collision of a hydrogen-like atom with another system (a nucleus, atom, electron, etc.), can be solved in terms of a Born expansion where the first term of the series is the leading one contributing to the differential cross section. As an example, let's consider the collision of an atom with a center of force field described by a potential  $V(\mathbf{r})$ . The cross section for the atom transition from an initial bound state,  $(n_1, l_1, m_1)$ , to a final bound state  $(n_2, l_2, m_2)$  can be expressed in terms of the atomic form factors  $F_{n_1 l_1 m_1}^{n_2 l_2 m_2}(\mathbf{q})$  [3]:

$$\sigma_{n_1 l_1 m_1}^{n_2 l_2 m_2} = \frac{1}{4\pi\beta^2} \int_0^\infty |\tilde{V}(\mathbf{q})|^2 |F_{n_1 l_1 m_1}^{n_2 l_2 m_2}(\xi_1 \mathbf{q}) - F_{n_1 l_1 m_1}^{n_2 l_2 m_2}(\xi_2 \mathbf{q})|^2 q \, dq, \quad (2)$$

$$F_{n_1 l_1 m_1}^{n_2 l_2 m_2}(\mathbf{q}) = \int \psi_{n_2 l_2 m_2}^*(\mathbf{r}) e^{i\mathbf{q}\mathbf{r}} \psi_{n_1 l_1 m_1}(\mathbf{r}) \, d\mathbf{r}, \quad (3)$$

where  $\tilde{V}(\mathbf{q})$  is the Fourier transform of the center potential  $V(\mathbf{r})$ ,  $\beta$  is the velocity of the atom and  $\mathbf{q}$  the transferred momentum in the collision. The coefficients  $\xi_1$  and  $\xi_2$  are related to the masses of the particles of the hydrogen-like atom by  $\xi_1 = m_1/(m_1 + m_2)$  and  $\xi_2 = -m_2/(m_1 + m_2)$ . Finally,  $\psi_{nlm}$  is the wave function of the hydrogen-like atom.

The total cross section is given by:

$$\sigma_{nlm}^{\text{total}} = \frac{1}{2\pi\beta^2} \int_0^\infty |\tilde{V}(\mathbf{q})|^2 (1 - F_{nlm}^{nlm}(\mathbf{q})) q \, dq. \quad (4)$$

The atomic form factors given by Eq. (3) appear in the first Born approximation of any cross section calculation in which an atom is involved. The original motivation for this work came from the need of the DIRAC collaboration [4, 5] at CERN [6] to have a computer implementation of generic hydrogen-like atomic form factors. DIRAC aims to measure the lifetime of dimesonic  $\pi^+\pi^-$  atoms, which are produced in the collision of the CERN PS proton beam with a fixed target. After creation,  $\pi^+\pi^-$  atoms go across the target material before breaking up in two

#### Restrictions on the complexity of the problem

For a non-relativistic collision the Born approximation is safely valid if the kinetic energy of the projectile in the laboratory frame obeys [3]:

$$\frac{p^2}{2M} \gg -E, \quad (1)$$

where  $E$  is the bound energy of the hydrogen-like atom initial state. For the case of relativistic collisions it has been shown that multi-photon exchange can lead to significant corrections in the hydrogen-like atom collision [8]. However, the relativistic calculation also involves the atomic form factors<sup>1</sup> and for many small and medium  $Z$  atoms in  $n \leq 10$  bound states the discrepancies are less than 10%.

<sup>1</sup> The useful expressions for the multi-photon exchange cross sections as a function of the atomic form factors can be found in [8].

charged pions or getting disintegrated in two neutral pions. To know from which atomic state the atom gets broken (ionized) it is essential to compute the transition probabilities between two different atomic states, and this requires obviously the computation of discrete–discrete atomic form factors. A detailed explanation of  $\pi^+\pi^-$ -physics in DIRAC framework can be found in [9].

## 2. Analytical expression for the discrete form factors

For hydrogen-like atoms it is possible to perform the integral (3) and give an analytical general expression for the atomic form factors [7]:

$$F_{n_1, l_1, m_1}^{n_2, l_2, m_2}(\mathbf{q}) = N \sum_{k=0}^{k_m} H_k \sum_{p=0}^{p_m} D_p \Delta^{L-2p} \omega^{L-p+2} [C_k^{(L+2, p)}(z) + C_{k-1}^{(L+2, p)}(z)], \quad (5)$$

where

$$N = \frac{(2a)^{l_1+1} (2b)^{l_2+1}}{n_1 + n_2} \sqrt{\lambda_1 \lambda_2 \frac{\Gamma(n_{r_1} + 1) \Gamma(n_{r_2} + 1)}{\Gamma(n_{r_1} + \lambda_1 + 1) \Gamma(n_{r_2} + \lambda_2 + 1)}}, \quad (6)$$

$$a = \frac{n_2}{n_1 + n_2}, \quad b = \frac{n_1}{n_1 + n_2}, \quad k_m = n_{r_1} + n_{r_2}, \quad p_m = \min(l_1, l_2),$$

$$\lambda_1 = 2l_1 + 1, \quad \lambda_2 = 2l_2 + 1, \quad n_{r_1} = n_1 - l_1 - 1, \quad n_{r_2} = n_2 - l_2 - 1.$$

Concerning  $D_p$ :

$$D_p = 2^{L+1} \Gamma(L - p + 2) \sum_{s=p}^{p_m} (-1)^{s-p} \Gamma(p + 1) \binom{s}{p} \binom{L - s + \frac{1}{2}}{p} A_s, \quad (7)$$

where

$$A_s = i^L (-1)^{s+m_2} \sqrt{\frac{4\pi}{(2l+1)}} \langle l_1, l_2, 0, 0 | l, 0 \rangle \langle l_1, l_2, m_1, -m_2 | l, m \rangle Y_{l, m}(\theta_q, \phi_q), \quad (8)$$

$$L = l_1 + l_2, \quad l = L - 2s.$$

The coefficients  $H_k$  are given by:

$$H_k = (-1)^{k+n_{r_2}} \binom{n_{r_1} + n_{r_2}}{n_{r_2}} \binom{n_{r_1} + n_{r_2}}{k}^{-1} Q_k^{(n_{r_2}, n_{r_1})} Q_{\bar{k}}^{(n_{r_1} + \lambda_1, n_{r_2} + \lambda_2)}, \quad (9)$$

$$\bar{k} = n_{r_1} + n_{r_2} - k.$$

The  $Q_n^{(\mu, \nu)}$  of Eq. (9) are expressed in terms of the Jacobi polynomial as:

$$Q_n^{(\mu, \nu)} = P_n^{(\mu-n, \nu-n)}(b-a), \quad (10)$$

which can be written as a series:

$$P_n^{(\alpha, \beta)}(x) = \sum_{m=0}^n \frac{1}{2^n} \binom{n+\alpha}{m} \binom{n+\beta}{n-m} (x-1)^{n-m} (x+1)^m. \quad (11)$$

Finally, the  $C_k$  in (5) are the generalized Gegenbauer functions, defined by:

$$C_k^{(\lambda, p)}(z) = \frac{\Gamma(k+2\lambda)}{\Gamma(k+1)\Gamma(2\lambda)} \sum_{i=0}^k \frac{(-k)_i (2\lambda+k)_i (\lambda-p)_i}{(\lambda+1/2)_i \lambda_i} \frac{1}{i!} \left(\frac{1-z}{2}\right)^i, \quad (12)$$

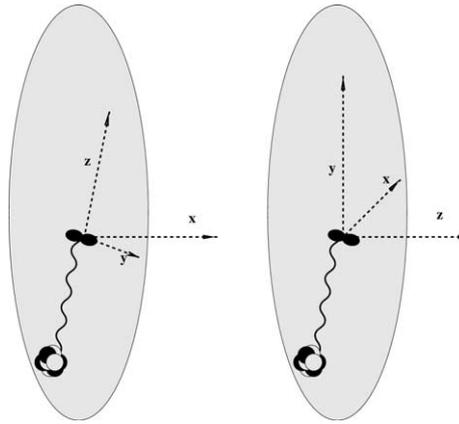


Fig. 1. Choice of axis. As usual  $z$  is the quantization axis.

where anything with the subscript  $i$  means the product  $\alpha_i = (\alpha + i - 1)(\alpha + i - 2) \cdots \alpha$ . Finally the dependence on  $q$  is given by:

$$\Delta = \frac{qn_1n_2}{n_1 + n_2}, \quad \omega = \frac{1}{1 + \Delta^2}, \quad z = 1 - 2\omega.$$

The direction of the quantization axis depends on the choice of  $Y_{lm}(\theta_q, \phi_q)$  in the expression for  $A_s$ . If the direction of  $\mathbf{q}$  is taken as the quantization axis we have:

$$Y_{lm}(0, \phi) = \delta_{m0} \sqrt{\frac{2l+1}{4\pi}}. \quad (13)$$

A more useful convention, nevertheless, would be to choose the quantization axis parallel to the collision direction. This is particularly convenient when the initial momentum of the flying atom is much larger than the transferred momentum in the collision. In this case the quantization axis remains almost unchanged in successive collisions. Since the transferred momentum is almost perpendicular to this axis choice ( $q \approx q_{\perp}$ , and  $\theta_q \approx \pi/2$ ), we write:

$$Y_{l,m}\left(\frac{\pi}{2}, \phi\right) = (-1)^m 2^{-l} e^{im\phi} \cos\left(\frac{\pi}{2}(l+m)\right) \frac{\sqrt{(l+m)!(l-m)!}}{\Gamma(\frac{l-m}{2}+1)\Gamma(\frac{l+m}{2}+1)} \sqrt{\frac{2l+1}{4\pi}}. \quad (14)$$

Some tables of atomic form factors have been published for the first choice of axis [3,10], and they are in good agreement with the results obtained using the generic expression given by (5).

### 3. Description of the program

We provide a FORTRAN implementation of the discrete atomic form factors as given by Eq. (5), and the axis choice of (14). This is done by means of a double precision function, DIFOFA, which should be called by the user main program with the following arguments:

$$\text{DIFOFA}(n_1, l_1, m_1, n_2, l_2, m_2, q), \quad (15)$$

- $n_1, l_1$  and  $m_1$  are integers representing the quantum numbers of the initial atomic state.
- $n_2, l_2$  and  $m_2$  are integers representing the quantum numbers of the final atomic state.
- $q$ , is a double precision argument representing the momentum transferred in the collision in *atomic units*:  $q_{(\text{atomic units})} = q/(\mu c \alpha)$ , where  $\alpha$  is the fine structure constant,  $\mu$  is the reduced mass of the hydrogen-like atom and  $\mu = m_1 m_2 / (m_1 + m_2)$ .

Table 1

---

DOUBLE PRECISION FUNCTION DIFOFA( N1, L1, M1, N2, L2, M2, Q )	
DIFOFA	Returns the discrete--discrete atomic form factors
N1, L1, M1	Are integers representing the quantum numbers of the initial atomic state.
N2, L2, M2	Are integers representing the quantum numbers of the final atomic state.
Q	Is a double precision argument representing the momentum transferred in the atomic collision in atomic units:  $Q(\text{atomic\_units}) = Q(\text{MeV}) / \text{Mu}(\text{MeV}) / \text{alpha}$ where Mu(MeV) is the reduced mass of the hydrogen-like atom and 'alpha' is the fine structure constant.

---

DIFOFA internally calls a number of functions. They are not intended to be directly called by the user, but they could also be used by other programs in a straight forward way.

- DOUBLE PRECISION FUNCTION EUGAMM(N), is the Euler gamma function for an integer argument.
- DOUBLE PRECISION FUNCTION GEGENF(L,P,K,Z), are the generalized Gegenbauer functions given by Eq. (12).
- DOUBLE PRECISION FUNCTION DJACPO(ALFA,BETA,N,X), are the Jacobi polynomials given by Eq. (11).
- DOUBLE PRECISION FUNCTION DBINOM(X,K) are the binomial coefficients. The code is taken directly from the CERN program library CERNLIB [11].
- DOUBLE PRECISION FUNCTION DCLEBG(A1,B1,C1,X1,Y1,Z1) are the Clebsch–Gordan coefficients. The code is also taken directly fro the CERN program library CERNLIB [11].

The header of the source code looks as follows (see Table 1).

#### 4. Test run input and output

The best way to illustrate the output of the program is to plot the value of the atomic form factors versus the transferred momentum. As an example, we plot in Fig. 2 the form factors for 4 different transitions. The transferred momentum is measured in atomic units.

From Eq. (3) we clearly see that:

$$F_{n_1 l_1 m_1}^{n_2 l_2 m_2}(0) = \int \psi_{n_2 l_2 m_2}^*(\mathbf{r}) \psi_{n_1 l_1 m_1}(\mathbf{r}) \mathbf{d}\mathbf{r} = \delta_{n_1 n_2} \delta_{l_1 l_2} \delta_{m_1 m_2} \quad (16)$$

therefore the discrete–discrete atomic form factors evaluated at zero transferred momentum should be either 0 or 1, as it can be verified in Fig. 2.

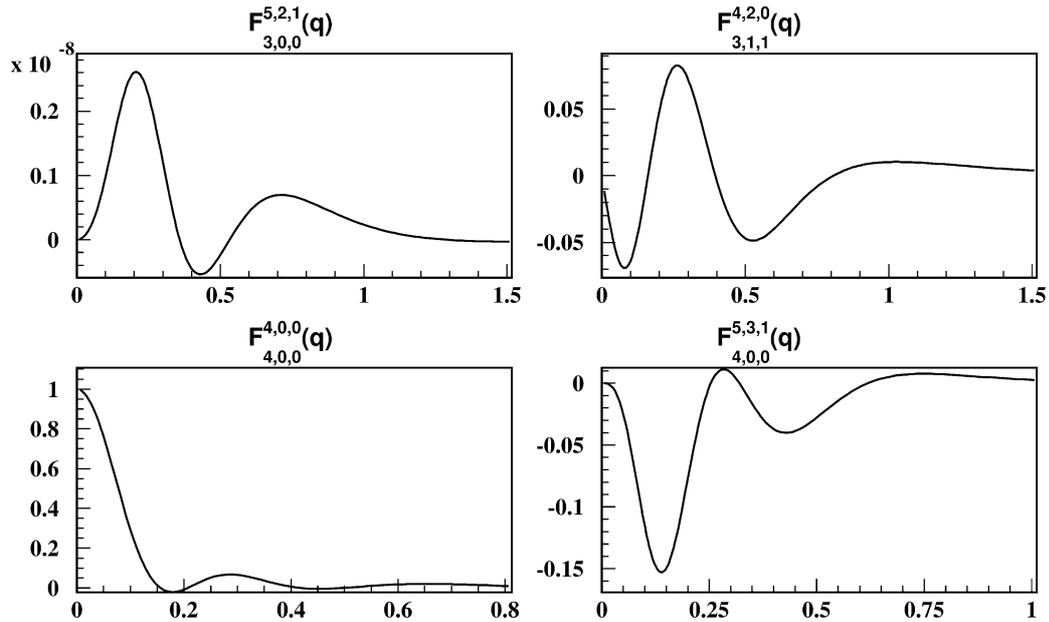


Fig. 2. Plots of discrete–discrete atomic form factors for 4 different transitions versus the transferred momentum measured in atomic units.

To determine the range of atomic quantum numbers where our program gives reliable results we provide a test program that computes the absolute difference  $|F_{n,l,m}^{n,l,m}(0) - 1|$  for all the states up to those with  $n = 10$ . The results are shown in Appendix A. However, we have performed this test for a wider range of quantum numbers paying special attention to the least favorable case ( $l = 0, m = 0$ ). It has been observed that if  $n \leq 7$  the program works with a high level of precision. For  $n = 12$  the deviation from the correct value is of the order of 1%, and for  $n > 13$  the results begin to be senseless. For any other case the program works with almost any reasonable value of the quantum numbers. As an example, for the most favorable case ( $l = n - 1, m = 0$ ), the value of  $|F_{n,n-1,0}^{n,n-1,0}(0) - 1|$  remains satisfactorily small up to  $n \leq 30$ .

Finally, we have prepared another main program which calculates the cross section of fast electrons by an hydrogen atom for any state up to  $n = 11$ . The expression for this scattering cross section is given by [12]:

$$\sigma_{nlm} = \int_0^{\infty} 8\pi (1 - F_{nlm}^{nlm}(q)) \frac{dq}{q^3}. \quad (17)$$

The integration is performed with the CERNLIB routine DADAPT [11] after the change:

$$q \rightarrow \frac{x}{1-x} \quad (18)$$

that allows transforms the semi-infinite interval  $(0, \infty)$  into  $(0, 1)$ . The output is also shown in Appendix A.

## Appendix A. Test results

### A.1. Test result 1

We describe how to build and run the test program that computes the value of  $|F_{n,l,m}^{n,l,m}(0) - 1|$  for all the bound states up to  $n = 10$ . We also show the final display output.

Command line:

```
> make ffdiff
> ./ffdiff
```

Screen output:

```
** ***** **
** **
** This Output File gives us the **
** **
** absolute value of the result **
** **
** of subtracting 1. to the form **
** **
** form factor of a state at the **
** **
** origin. The expected result is **
** **
** 0. **
** ***** **
```

N	L	M	FFactor(0)-1.
1	0	0	0.00E+00
2	0	0	0.00E+00
2	1	0	0.22E-15
2	1	1	0.22E-15
3	0	0	0.10E-13
3	1	0	0.44E-15
3	1	1	0.44E-15
3	2	0	0.67E-15
3	2	1	0.67E-15
3	2	2	0.67E-15
4	0	0	0.74E-13
4	1	0	0.44E-15
4	1	1	0.44E-15
4	2	0	0.00E+00
4	2	1	0.00E+00
4	2	2	0.00E+00
4	3	0	0.33E-15
4	3	1	0.00E+00
...			
10	8	5	0.87E-14
10	8	6	0.99E-14

10	8	7	0.83E-14
10	8	8	0.12E-13
10	9	0	0.56E-14
10	9	1	0.56E-14
10	9	2	0.56E-14
10	9	3	0.36E-14
10	9	4	0.47E-14
10	9	5	0.47E-14
10	9	6	0.53E-14
10	9	7	0.36E-14
10	9	8	0.56E-14
10	9	9	0.56E-14

---

### A.2. Test result 2

This is the way to build and run the test program that computes fast electrons versus hydrogen atoms scattering. The program output is also shown.

Command line:

```
> make ffcsecc
> ./ffcsecc
```

Screen output:

```
** ***** **
**
** This Output File gives us the **
** result of the elastic cross **
** section of fast electrons **
** against hydrogen atoms **
** scattering in the First Born **
** approximation. **
** Cross sections and Err. in **
** square Bohr radius units **
** a0**2= 0.280 10**-20 m**2 **
** ***** **
```

N	L	M	Cross Secc.	Err.
1	0	0	7.33	0.00
2	0	0	124.53	0.00
2	1	0	46.50	0.00
2	1	1	109.15	0.00
3	0	0	639.11	0.00
3	1	0	298.27	0.00
3	1	1	704.09	0.00
3	2	0	219.41	0.00
3	2	1	337.32	0.00
3	2	2	536.82	0.00
4	0	0	2029.93	0.00
4	1	0	1017.18	0.00
4	1	1	2404.81	0.00
4	2	0	884.08	0.00
4	2	1	1363.68	0.00
4	2	2	2174.17	0.00
4	3	0	678.12	0.00
4	3	1	866.82	0.00
...				
10	8	5	49453.51	21.91
10	8	6	56553.16	29.91
10	8	7	64343.01	34.55
10	8	8	72794.42	7.86
10	9	0	24933.60	6.24
10	9	1	25834.98	6.33
10	9	2	28037.93	6.62
10	9	3	31237.44	7.17
10	9	4	35230.79	8.11
10	9	5	39879.30	9.74
10	9	6	45088.87	12.60
10	9	7	50798.16	17.71
10	9	8	56970.20	26.02
10	9	9	63586.26	35.89

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