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Elastic – Elastic scattering of electrons from ions and atoms

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Abstract

A computer program, *Elastic*, is presented which calculates the elastic scattering cross section as a function of scattering angle for electrons colliding with ions or atoms. The scattering is computed in an independent particle approach through calculation of the scattering phase shifts for an electron encountering a parameterized model potential. The functional form of the potential implemented is approximately valid for all ions and atoms and has parameters that are based on a fit of Hartree–Fock orbital energies (R.H. Garvey, C.H. Jackman, A.E.S. Green, Phys. Rev. A 12 (1975) 1144). The user could easily modify the program to utilize other forms however. An auxiliary program, *Green-pot*, is included which computes the parameters of the Garvey et al. potential for use in *Elastic*, for display and analysis of the potential, and for use in other applications. © 1998 Elsevier Science B.V.

PACS: 34.80.Bm; 34.80.-i; 34.20.Cf

Keywords: Elastic; elastic scattering; differential cross section; electron–atom scattering; electron–ion scattering; electron–atom potential; electron–ion potential

PROGRAM SUMMARY

Title of program: *Elastic*, *Green-pot*

Catalogue identifier: ADJH

Program Summary URL:

<http://www.cpc.cs.qub.ac.uk/cpc/summaries/ADJH>

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland

Licensing provisions: none

Computers: HP/755, SGI Power Challenge, Dec alpha PC, IBM PC

Operating systems under which the program has been tested: HPUX 9.x, 10.x, IRIX 7.x, LINUX, OS/2

Programming language used: f77, g77

Memory required to execute with typical data: 2500 words

No. of bits in a word: 64

Has the code been vectorised?: yes

No. of bytes in distributed program, including test data, etc.: 30772

Distribution format: ASCII

Keywords: elastic, elastic scattering, differential cross section, electron–atom scattering, electron–ion scattering, electron–atom potential, electron–ion potential

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Nature of physical problem

In an independent particle approach, the program describes the elastic scattering of an electron from a model potential representing any atom or ion.

Method of solution

The program solves the radial Schrödinger equation by the log derivative method of B.R. Johnson [1] for a model potential to obtain scattering phase shifts and angular differential cross sections for elastic scattering. An auxiliary program computes the required input values for a parameterized Hartree-Fock, independent particle model potential of R.H. Garvey, C.H. Jackman, and A.E.S. Green [2].

Restrictions on the complexity of the problem

Single channel approximation (i.e., neglect of electron exchange and coupling to inelastic channels) for elastic scattering of electrons from arbitrary ions and atoms.

Typical running time

Less than five seconds.

References

- [1] B.R. Johnson, *J. Comput. Phys.* 13 (1973) 445.
- [2] R.H. Garvey, C.H. Jackman, A.E.S. Green, *Phys. Rev. A* 12 (1975) 1144.

LONG WRITE-UP

1. Introduction

The elastic scattering of an electron from an atom or ion is a ubiquitous phenomenon occurring in a wide range of physical contexts such as in astrophysical or atmospheric environments, fusion reactors, technical plasmas used for modifying or machining materials such as semiconductors, and common devices such as fluorescent lighting. Thus, it would be convenient to have a simple, flexible, program to compute the elastic differential cross section from an arbitrary atom or ion for use in these applications or in fundamental studies. That is the objective addressed by the presently described code, *Elastic*, and its associated auxiliary code, *Green-pot*.

Early versions of these codes were developed to serve as input to a binary encounter approximation used to describe the ejected electron spectrum in ion-atom collisions. In particular, in the early 1990s it was discovered that the forward binary peak exhibited a seemingly anomalous enhancement when the impacting ion was only partially stripped, compared to fully stripped ion-impact [1,2]. It was shown that this enhancement resulted from the enhanced backward scattering of the released target electron in the screened potential of the projectile (backward scattering in the projectile frame leads to forward scattering in the target or laboratory frame) [3–5]. Similar theoretical interpretations were made essentially contemporaneously by several other groups (e.g., [6–8]).

In addition, this code was used to explain the origins of what at the time was considered to be a completely unrelated phenomenon, an oscillation superimposed on the binary peak at intermediate ejection angles (e.g., [9]). It was shown that, similarly to the enhancement of the binary peak at forward angles for partially stripped ion-impact, the oscillation arises from the diffractive elastic scattering of the target electron by the partially stripped projectile [10]. In this case, the deep diffractive minima which survive the averaging over the Compton profile of the target electron are largest when the ratio of the projectile ionic charge to its nuclear charge is small. That is, for heavy projectiles such as iodine or uranium in relatively low charge states, production of the oscillatory binary peak is enhanced.

Other applications of this code are easy to envision. Recently of interest has been the direct investigation of elastic scattering of electrons by ions [11]. Also, certain experiments require knowledge of the elastic cross section to estimate backgrounds for inelastic channel measurements [12]. Applications such as those encountered in modeling plasma environments should in general also benefit from the availability of a code for arbitrary ions and atoms. This will allow the calculation of estimates of the elastic scattering cross sections, which can play a crucial role in the energy and momentum transport in the plasma.

Thus, presented here is a code to compute such elastic differential cross sections for any ion or atom (with nuclear charge less than 100) based on the solution of the radial Schrödinger equation for electron scattering in a (parameterized) model potential. In the following sections we describe the theoretical method (Section 2) and the use of the code and its auxiliary code (Sections 3–5). Atomic units ($\hbar = e = m_e = 1$) are used throughout except where noted. For the user who requires more detailed or sophisticated treatment of electron–ion/atom scattering (e.g., with inclusion of exchange and inelastic channels) descriptions of codes may be found in the present special issue. These include works based on the “convergent close-coupling” (CCC) approach of Bray and Stelbovics [13], the “R-matrix with pseudo-states” (RMPS) method of Bartschat et al. [14], and the “intermediate energy R-matrix” approach outlined by Burke et al. [15].

2. Theoretical method

Though the calculation of the elastic differential cross section for the scattering of an electron in a potential is rather common (see, e.g., [16,17]), scattering from an ion has the complication that the long range Coulomb interaction requires a different, combined treatment. To accomplish this, we integrate the radial Schrödinger equation (using the efficient and accurate procedure introduced by Johnson [18]) for the non-Coulomb part of the ionic potential out to some large enough distance for each angular momentum. At this matching radius use is made of the analytic form of the radial wavefunction and the scattering phase shifts as a function of the radial wavefunction and its derivative. The elastic differential cross section is then derived from a properly weighted sum of the partial wave contributions.

The same procedure can be applied to electron–atom scattering, simply by setting the long range Coulomb interaction to zero. In this approach, an independent electron model is assumed, neglecting the multichannel nature of the collision, spin-orbit effects, polarization, and electron exchange. The computations are carried out in the non-relativistic limit.

Specifically, for an electron scattering from an ion of charge q and nuclear charge Z , the elastic differential cross section for scattering into a solid angle element $d\Omega$ as a function of the center of mass scattering angle θ is

$$\frac{d\sigma}{d\Omega}(\theta) = |f_c(\theta) + f_{nc}(\theta)|^2, \quad (1)$$

where the scattering amplitude is composed of both a Coulomb (c) and non-Coulomb (nc) part. The Coulomb amplitude is given by

$$f_c = \frac{-\alpha \exp(2i\sigma_0)}{2\mu v \sin^2(\theta/2)} \exp[-i\alpha \log(\sin^2(\theta/2))], \quad (2)$$

where $\alpha = -q/v$ is the so-called Coulomb factor, v is the collision velocity, $\sigma_l = \arg(\Gamma(l+1+i\alpha))$ is the Coulomb phase shift, and μ is the reduced mass of the electron–ion system. Typically, $\mu = 1$ and θ is the scattering angle in the frame of the heavy ion. For the non-Coulomb part, a partial wave expansion is made, i.e.

$$f_{nc} = \frac{1}{2ik} \sum_{\ell=0}^{\ell_{\max}} (2\ell+1) e^{2i\sigma_\ell} (e^{2i\delta_\ell} - 1) P_\ell(\cos \theta), \quad (3)$$

where $k = \mu v$, ℓ is the angular momentum quantum number, δ_ℓ is the non-Coulomb phase shift, and P_ℓ the associated Legendre polynomial of order ℓ . In practice, the sum is evaluated up to a maximum quantum number ℓ_{\max} such that $\delta_{\ell_{\max}} \approx 0$ (e.g., $\delta_{\ell_{\max}} < 0.001$).

For an arbitrary potential, there is of course no analytic solution of the Schrödinger equation, and consequently we find it through numerical integration. The radial Schrödinger equation is

$$u_\ell''(r) + [k^2 - 2\mu V - \ell(\ell + 1)/r^2]u_\ell(r) = 0, \quad (4)$$

where r is the radial coordinate, $u_\ell(r)$ is the radial wavefunction of angular momentum ℓ , $V(r)$ is the interaction potential, and the primes indicate the derivative operation with respect to r . The general solution of this differential equation behaves asymptotically as

$$\lim_{r \rightarrow \infty} u_\ell = c_1 F_\ell(\alpha, kr) + c_2 G_\ell(\alpha, kr), \quad (5)$$

where F_ℓ and G_ℓ are regular and irregular spherical Coulomb functions. Defining the logarithmic derivative

$$L = \frac{u_\ell'}{u_\ell}, \quad (6)$$

one can show that

$$\tan \delta_\ell = \frac{(L/k)F_\ell - F_\ell'}{G_\ell' - (L/k)G_\ell}. \quad (7)$$

We utilize this expression by numerically integrating the radial equation out to some large distance, finding u_ℓ and u_ℓ' , and evaluating the asymptotic form of the spherical Coulomb functions. This procedure is simplified by using Johnson's [18] scheme which utilizes the logarithmic derivative directly, by first transforming the Schrödinger equation to the Riccati equation. His method has the benefit of yielding a numerical error term one order smaller than that of the widely used Numerov method.

In order to represent the widest possible range of ions and atoms with a single form of the potential, we have used a parametrized Hartree–Fock model potential derived and tabulated by Garvey et al. [19] for any ion or atom with $2 < Z < 54$. The potential has the form

$$V(r) = [(N - 1)(1 - \Omega(r)) - Z]/r, \quad (8)$$

where

$$\Omega(r) = [(\eta/\xi)(e^{\xi r} - 1) + 1]^{-1}, \quad (9)$$

and, following the notation of Garvey et al. [19], where $(N - 1)$ is the number of electrons present in the ion or atom and the screening parameters, $\eta(N, Z)$ and $\xi(N, Z)$, have been tabulated. We note that for an electron scattering from an ion Z^{q+} , N , Z , and q are related as $N = Z - q + 1$. Some values of these parameters (i.e., for $N = 38, 40, 43, 45, 47, 49, 51$, and 53) were not tabulated by Garvey et al., but following their suggestion we have interpolated them since they are smoothly varying functions for large N . This smooth behavior has also lead us to *extrapolate* these values for $Z, N > 54$ so that the code is capable of estimations for heavy ions and atoms as well. The user should note that even though we have found reasonable results for our applications using this extrapolation, its appropriateness should be evaluated for other applications. We have also extrapolated the potential for neutral atoms using $N = Z + 1$. In addition, we have approximated parameters for another possibly important case, atomic hydrogen, which was obviously not part of Garvey et al.'s Hartree–Fock survey. In this case, we varied the values of the parameters to match reasonably well the exact electrostatic potential experienced by an electron interacting with the ground state of hydrogen. Users should also examine for themselves if these simple and imperfect approximations are sufficient for their application. In fact, the routine that evaluates the potential could be easily adapted to any other desired functional form.

3. Program description

The program *Green-pot* has a very simple structure. After defining statement functions which implement the functional form of the Garvey et al. [19] potential, the program calls the subroutine *param* in order to determine the proper parameters of this potential. Finally, these parameters are written to the standard output and a file, *green-pot.out*, is written containing a tabulation of the model potential as a function of radius along with other useful diagnostic information (e.g., the Coulomb potential for a bare ion of charge q , and the differences between this potential and the model potential).

The following outlines the structure and dependencies in the program *Elastic*:

program elastic – the main calling program unit

- (i) **subroutine readit** – reads the input
- (ii) **loop over angular momenta** – integrate the radial Schrödinger equation for each required value of the electron's angular momentum (l_{\min} to l_{\max}) on the radial grid from r_{start} to r_{end0}
 - **subroutine pot** – evaluates the model potential at the given radius
- (iii) **calculation of the phase shifts**
 - **subroutine cwf** – compute the Coulomb wavefunctions for all angular momenta up to l_{\max}
 - **function cgamma** – complex Gamma function
 - **subroutine hyper** – regular and irregular hypergeometric functions and their derivatives
- (iv) **loop over angular momenta** – calculate phase shifts as a function of angular momentum and the total cross section for neutral targets (atoms)
- (v) **loop over angles** – compute and write differential cross sections
 - **function cgamma** – complex Gamma function
 - **function pl** – Legendre polynomials
 - **function zeff** – effective charge for use in Born approximation
 - **subroutine romba** – Romberg integration of function **fint**
 - **close, stop, end**

4. Input and output

To determine the appropriate values of the model potential parameters, the user should first run the program *Green-pot*, or manually calculate them from the original Garvey et al. [19] tabulation. One inputs q and Z and the program outputs to the screen the values of ξ and η . These parameters, q , Z , ξ , and η , are required input for the elastic scattering code. Also required is the range at which the model potential becomes negligibly different from the Coulomb potential. Since the model potential contains an exponential function, it is numerically convenient to switch at this radius to the Coulomb potential. The code *Green-pot* makes a suggestion for this radius by computing the difference between the model and Coulomb potentials as a function of radius, and the difference between their derivatives, checking that the differences reach tolerances set in the code.

Green-pot also writes to a file *Green-pot.out* which contains a tabulation as a function of a radial grid of the model potential, the Coulomb potential for a bare charge equal to the ionic charge q , and the difference between these two potentials. This file facilitates plotting of the potential and evaluation of the recommended range.

The input to *Elastic* consists of the impacting electron energy (en) in eV, the matching radius (r_{end0}) at which point to switch from the numerical solution to the asymptotic solution, the step ($spac$) for the numerical integration, the minimum, maximum, and step in angular momentum (l_{\min} , l_{\max} , l_{spc}) for the partial wave summation, the Garvey et al. model potential parameters (q_{mod} , z_{mod} , ξ , η , r_{mod}), and finally, a flag ($iborn$) to allow calculation of the result in the first Born approximation. The latter option is useful for

comparisons. Of the other inputs not obvious from previous discussions is `rend0` which should be chosen such that the potential has reached its asymptotic form (i.e., `rend0` > `rmod`) so the wavefunction can justifiably be represented as the assumed linear combination of regular and irregular Coulomb functions, and such that the routine used to compute the asymptotic hypergeometric functions is correct. A recommended value for `rend0` is 10 a.u./ k and certainly should not be smaller than `rmod`, the range of the model potential obtained from *Green-pot* or the user's inspection. The radial step `spac` for the numerical integration can be varied to test for convergence of the result, and we find that a reasonable starting estimate is 0.001 a.u.

Elastic outputs an echo of the input variables, and then as a function of partial wave (ℓ) both the non-Coulomb and Coulomb phase shifts. The user can judge from the convergence of these phase shifts whether or not `lmax` should be increased. Next, the total elastic cross section (`tcs`) is printed in a.u. for the case of neutral targets (i.e., atoms), and then either the "exact" (i.e., from the numerical integration) or Born approximation differential elastic cross sections as a function of the scattering angle in degrees. For comparison, two other cross sections are printed as well. These are the Rutherford cross section for scattering from a bare charge of magnitude equal to either the ionic charge q (denoted Rutherford- q) or nuclear charge (Rutherford- Z).

5. Test run description

The input and output of a simple test of the pair of programs is reproduced below. In this test, interactive I/O is made at the console to run *Green-pot* to determine the model potential parameters for an electron interacting with Xe^+ . Thus, the user enters the values 1. and 54. for the target's ionic and nuclear charge, respectively. The program then prints to the screen the appropriate model potential parameters and an estimate of the range over which the model potential significantly deviates from the Coulomb potential of a bare charge q . The output file *green-pot.out* is also written which tabulates the model potential as a function of radius, along with the Coulomb potential, the difference between the model and Coulomb potentials, and the difference between their derivatives with respect to radius.

To run the code *Elastic* to obtain the elastic scattering cross section for a 1000 eV electron from Xe^+ , the file *elastic.in* is edited to include the model potential parameters output from *Green-pot*, the electron energy, and several other user selectable options. For example, one may chose to use the Born approximation rather than the generally more accurate numerical integration of the radial Schrödinger equation. Also one can chose the radial step size and ending distance for the numerical integration and the range of angular momentum. The values given in the example yield good convergence in these variables (radial step and distance, and angular momentum range). The output of the code is then written to *elastic.out* which echoes the input variables and then tabulates phase shifts so the user can see and check the convergence of the the non-Coulomb phase shifts. Finally, the code writes out as function of scattering angle the differential cross sections as described in the section on I/O above.

Acknowledgements

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References

- [1] P. Richard, D.H. Lee, T.J.M. Zouros, J.M. Sanders, J.L. Shinpaugh, *J. Phys. B* 23 (1990) L213.
- [2] D.H. Lee, P. Richard, T.J.M. Zouros, J.M. Sanders, J.L. Shinpaugh, H. Hidmi, *Phys. Rev. A* 41 (1990) 4816.
- [3] R.E. Olson, C.O. Reinhold, D.R. Schultz, *J. Phys. B* 23 (1990) L455.
- [4] C.O. Reinhold, D.R. Schultz, R.E. Olson, *J. Phys. B* 23 (1990) L591.
- [5] D.R. Schultz, R.E. Olson, *J. Phys. B* 24 (1991) 3409.
- [6] T. Quinteros, J.F. Reading, *Nucl. Instr. & Methods B* 53 (1991) 363.
- [7] R. Shingal, Z. Chen, K.R. Karim, C.D. Lin, C.P. Bhalla, *J. Phys. B* 23 (1990) L637.
- [8] K. Taulbjerg, *J. Phys. B* 23 (1990) L761.
- [9] C. Kelbch, S. Hagmann, S. Kelbch, R. Mann, R.E. Olson, S. Schmidt, H. Schmidt-Böcking, *Phys. Lett. A* 139 (1989) 304.
- [10] C.O. Reinhold, D.R. Schultz, R.E. Olson, C. Kelbch, R. Koch, H. Schmidt-Böcking, *Phys. Rev. Lett.* 66 (1991) 1842.
- [11] J.B. Greenwood, I.D. Williams, P. McGuinness, *Phys. Rev. Lett.* 75 (1995) 1062.
- [12] See, e.g., E.W. Bell et al., *Phys. Rev. A* 49 (1994) 4585;
Y-S. Chung et al., *Phys. Rev. A* 55 (1997) 2044.
- [13] I. Bray, A.T. Stelbovics, *Adv. At. Mol. Opt. Phys.* 35 (1995) 209.
- [14] K. Bartschat, E.T. Hudson, M.P. Scott, P.G. Burke, V.M. Burke, *J. Phys. B* 29 (1996) 115.
- [15] P.G. Burke, C.J. Noble, M.P. Scott, *Proc. Roy. Soc. A* 410 (1987) 289.
- [16] C.J. Joachain, *Quantum Collision Theory* (North-Holland, Amsterdam, 1983).
- [17] L.S. Rodberg, R.M. Thaler, *The Quantum Theory of Scattering* (Academic Press, New York, 1967).
- [18] B.R. Johnson, *J. Comput. Phys.* 13 (1973) 445.
- [19] R.H. Garvey, C.H. Jackman, A.E.S. Green, *Phys. Rev. A* 12 (1975) 1144.

TEST RUN OUTPUT

Input/Output for *Green-pot*Console I/O example (electron + Xe⁺)

Enter q, Z:

1.,54.

q, Z, xi, eta:

1.0 54.0 1.044 5.101

Estimated range:

14.1

green-pot.out

r	vm	vc	vm-vc	dvm-dvc
.0100	-5.1415E+03	-1.0000E+02	-5.0415E+03	5.2887E+05
.0200	-2.4523E+03	-5.0000E+01	-2.4023E+03	1.3146E+05
.0300	-1.5623E+03	-3.3333E+01	-1.5290E+03	5.7931E+04
.0400	-1.1215E+03	-2.5000E+01	-1.0965E+03	3.2239E+04
.0500	-8.6005E+02	-2.0000E+01	-8.4005E+02	2.0379E+04
.0600	-6.8797E+02	-1.6667E+01	-6.7130E+02	1.3959E+04
.0700	-5.6677E+02	-1.4286E+01	-5.5248E+02	1.0105E+04
.0800	-4.7721E+02	-1.2500E+01	-4.6471E+02	7.6166E+03
.0900	-4.0865E+02	-1.1111E+01	-3.9754E+02	5.9208E+03
.1000	-3.5468E+02	-1.0000E+01	-3.4468E+02	4.7160E+03
.2000	-1.2915E+02	-5.0000E+00	-1.2415E+02	9.8632E+02
.3000	-6.6495E+01	-3.3333E+00	-6.3162E+01	3.6809E+02
.4000	-4.0009E+01	-2.5000E+00	-3.7509E+01	1.7601E+02
.5000	-2.6374E+01	-2.0000E+00	-2.4374E+01	9.6934E+01
.6000	-1.8476E+01	-1.6667E+00	-1.6809E+01	5.8541E+01
.7000	-1.3522E+01	-1.4286E+00	-1.2093E+01	3.7737E+01
.8000	-1.0230E+01	-1.2500E+00	-8.9799E+00	2.5538E+01
.9000	-7.9451E+00	-1.1111E+00	-6.8340E+00	1.7945E+01
1.0000	-6.3037E+00	-1.0000E+00	-5.3037E+00	1.2994E+01
1.1000	-5.0914E+00	-9.0909E-01	-4.1823E+00	9.6414E+00
1.6000	-2.1252E+00	-6.2500E-01	-1.5002E+00	2.7796E+00
2.1000	-1.1091E+00	-4.7619E-01	-6.3291E-01	1.0265E+00
2.6000	-6.7636E-01	-3.8462E-01	-2.9175E-01	4.3373E-01
3.1000	-4.6455E-01	-3.2258E-01	-1.4197E-01	1.9880E-01
3.6000	-3.4938E-01	-2.7778E-01	-7.1597E-02	9.6048E-02
4.1000	-2.8092E-01	-2.4390E-01	-3.7016E-02	4.8103E-02
4.6000	-2.3688E-01	-2.1739E-01	-1.9487E-02	2.4715E-02
5.1000	-2.0648E-01	-1.9608E-01	-1.0401E-02	1.2940E-02
5.6000	-1.8418E-01	-1.7857E-01	-5.6114E-03	6.8739E-03
6.1000	-1.6699E-01	-1.6393E-01	-3.0537E-03	3.6930E-03
7.1000	-1.4177E-01	-1.4085E-01	-9.2280E-04	1.0938E-03
8.1000	-1.2374E-01	-1.2346E-01	-2.8467E-04	3.3239E-04
9.1000	-1.0998E-01	-1.0989E-01	-8.9194E-05	1.0293E-04
10.1000	-9.9038E-02	-9.9010E-02	-2.8290E-05	3.2336E-05
11.1000	-9.0099E-02	-9.0090E-02	-9.0620E-06	1.0277E-05
12.1000	-8.2648E-02	-8.2645E-02	-2.9265E-06	3.2972E-06
13.1000	-7.6337E-02	-7.6336E-02	-9.5162E-07	1.0661E-06
14.1000	-7.0922E-02	-7.0922E-02	-3.1125E-07	3.4702E-07
15.1000	-6.6225E-02	-6.6225E-02	-1.0232E-07	1.1360E-07
16.1000	-6.2112E-02	-6.2112E-02	-3.3783E-08	3.7368E-08


```

21.1000 -4.7393E-02 -4.7393E-02 -1.3939E-10 1.5213E-10
26.1000 -3.8314E-02 -3.8314E-02 -6.0927E-13 6.5948E-13
31.1000 -3.2154E-02 -3.2154E-02 -2.7409E-15 2.9751E-15
36.1000 -2.7701E-02 -2.7701E-02 .0000E+00 1.3553E-17
41.1000 -2.4331E-02 -2.4331E-02 .0000E+00 1.0842E-19
46.1000 -2.1692E-02 -2.1692E-02 .0000E+00 .0000E+00
51.1000 -1.9569E-02 -1.9569E-02 .0000E+00 5.4210E-20
56.1000 -1.7825E-02 -1.7825E-02 .0000E+00 -5.4210E-20
61.1000 -1.6367E-02 -1.6367E-02 .0000E+00 -5.4210E-20
66.1000 -1.5129E-02 -1.5129E-02 .0000E+00 -2.7105E-20

```

Input/Output for Elastic (1000 eV electron scattering from Xe⁺)

elastic.in

```

1000.          ! en, electron energy in eV
1.             ! rmu, electron-projectile reduced mass
0.            ! rstart, beginning of radial integ. (a.u.)
14.1          ! rend0, radius ending numerical integ. (a.u.)
1.e-3         ! space, numerical integration step (a.u.)
0,100,1       ! lmin, lmax, lspc
1.,54.,1.044,5.101,14.1 ! qmod, zmod, xi, eta, rmod
0             ! iborn, =0 numerical integ., =1 Born approx.

```

elastic.out

Elastic cross section by the Johnson method for potentials
of the Garvey et al. form

```

=====
impact energy: 3.67647E+01 a.u.
reduced mass: 1.00000E+00
rstart: .00000E+00 rend0: 1.41000E+01 spac: 1.00000E-03 a.u.
lmin: 0 lmax: 100 lspc: 1

```

```

nmod= 54 zmod= 5.40000E+01 xi= 1.04400E+00 eta= 5.10100E+00
rmod= 2.61000E+01 qmod= 1.00000E+00

```

```

1 = 0 phase shift = -1.3843352E+00 Coulomb phase shift= 6.6683272E-02
1 = 1 phase shift = 1.5948095E-01 Coulomb phase shift= -4.9411365E-02
1 = 2 phase shift = -1.5542503E+00 Coulomb phase shift= -1.0765493E-01
1 = 3 phase shift = 5.9668337E-02 Coulomb phase shift= -1.4650838E-01
1 = 4 phase shift = -9.7051023E-01 Coulomb phase shift= -1.7565489E-01
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1 = 19 phase shift = 9.9548651E-02 Coulomb phase shift= -3.4642034E-01

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*** ELASTIC CROSS SECTIONS ***

theta(deg)	dcs(a.u.)	Rutherford-q	Rutherford-Z
=====			
.0	7.9731E+15	7.9731E+15	2.3250E+19
1.0	9.7090E+03	7.9417E+03	2.3158E+07
2.0	1.1081E+03	4.9743E+02	1.4505E+06
3.0	4.2809E+02	9.8347E+01	2.8678E+05
4.0	2.3683E+02	3.1139E+01	9.0802E+04
5.0	1.4854E+02	1.2763E+01	3.7217E+04
6.0	9.8448E+01	6.1593E+00	1.7960E+04
7.0	6.7464E+01	3.3271E+00	9.7019E+03
8.0	4.7490E+01	1.9519E+00	5.6918E+03
9.0	3.4275E+01	1.2197E+00	3.5566E+03
10.0	2.5344E+01	8.0105E-01	2.3359E+03
11.0	1.9180E+01	5.4773E-01	1.5972E+03
12.0	1.4836E+01	3.8720E-01	1.1291E+03
13.0	1.1709E+01	2.8148E-01	8.2080E+02
14.0	9.4118E+00	2.0956E-01	6.1109E+02
15.0	7.6889E+00	1.5926E-01	4.6441E+02
16.0	6.3725E+00	1.2322E-01	3.5932E+02
17.0	5.3489E+00	9.6852E-02	2.8242E+02
18.0	4.5398E+00	7.7196E-02	2.2510E+02
19.0	3.8908E+00	6.2300E-02	1.8167E+02
20.0	3.3635E+00	5.0845E-02	1.4826E+02
21.0	2.9300E+00	4.1918E-02	1.2223E+02
22.0	2.5698E+00	3.4877E-02	1.0170E+02
23.0	2.2676E+00	2.9263E-02	8.5332E+01
24.0	2.0122E+00	2.4742E-02	7.2147E+01
25.0	1.7946E+00	2.1067E-02	6.1431E+01

26.0	1.6080E+00	1.8055E-02	5.2649E+01
27.0	1.4472E+00	1.5567E-02	4.5394E+01
28.0	1.3078E+00	1.3498E-02	3.9359E+01
29.0	1.1864E+00	1.1764E-02	3.4304E+01
30.0	1.0803E+00	1.0303E-02	3.0044E+01
31.0	9.8712E-01	9.0650E-03	2.6434E+01
32.0	9.0505E-01	8.0096E-03	2.3356E+01
33.0	8.3253E-01	7.1056E-03	2.0720E+01
34.0	7.6823E-01	6.3274E-03	1.8451E+01
35.0	7.1103E-01	5.6546E-03	1.6489E+01
36.0	6.6003E-01	5.0704E-03	1.4785E+01
37.0	6.1441E-01	4.5611E-03	1.3300E+01
38.0	5.7344E-01	4.1153E-03	1.2000E+01
39.0	5.3657E-01	3.7239E-03	1.0859E+01
40.0	5.0328E-01	3.3789E-03	9.8527E+00
41.0	4.7311E-01	3.0738E-03	8.9632E+00
42.0	4.4565E-01	2.8032E-03	8.1743E+00
43.0	4.2060E-01	2.5626E-03	7.4725E+00
44.0	3.9766E-01	2.3479E-03	6.8465E+00
45.0	3.7654E-01	2.1559E-03	6.2865E+00
46.0	3.5702E-01	1.9837E-03	5.7844E+00
47.0	3.3894E-01	1.8289E-03	5.3330E+00
48.0	3.2210E-01	1.6894E-03	4.9263E+00
49.0	3.0634E-01	1.5634E-03	4.5589E+00
50.0	2.9155E-01	1.4494E-03	4.2265E+00
51.0	2.7763E-01	1.3460E-03	3.9250E+00
52.0	2.6447E-01	1.2520E-03	3.6510E+00
53.0	2.5199E-01	1.1665E-03	3.4015E+00
54.0	2.4014E-01	1.0884E-03	3.1739E+00
55.0	2.2886E-01	1.0171E-03	2.9659E+00
56.0	2.1809E-01	9.5181E-04	2.7755E+00
57.0	2.0781E-01	8.9195E-04	2.6009E+00
58.0	1.9799E-01	8.3696E-04	2.4406E+00
59.0	1.8862E-01	7.8639E-04	2.2931E+00
60.0	1.7966E-01	7.3980E-04	2.1572E+00
61.0	1.7112E-01	6.9681E-04	2.0319E+00
62.0	1.6299E-01	6.5711E-04	1.9161E+00
63.0	1.5528E-01	6.2037E-04	1.8090E+00
64.0	1.4797E-01	5.8635E-04	1.7098E+00
65.0	1.4106E-01	5.5479E-04	1.6178E+00
66.0	1.3458E-01	5.2548E-04	1.5323E+00
67.0	1.2852E-01	4.9824E-04	1.4529E+00
68.0	1.2288E-01	4.7288E-04	1.3789E+00
69.0	1.1766E-01	4.4925E-04	1.3100E+00
70.0	1.1288E-01	4.2720E-04	1.2457E+00
71.0	1.0853E-01	4.0661E-04	1.1857E+00
72.0	1.0461E-01	3.8737E-04	1.1296E+00
73.0	1.0112E-01	3.6936E-04	1.0770E+00
74.0	9.8066E-02	3.5249E-04	1.0279E+00
75.0	9.5422E-02	3.3667E-04	9.8174E-01
76.0	9.3185E-02	3.2183E-04	9.3846E-01
77.0	9.1349E-02	3.0789E-04	8.9782E-01
78.0	8.9894E-02	2.9479E-04	8.5961E-01
79.0	8.8797E-02	2.8246E-04	8.2365E-01
80.0	8.8044E-02	2.7085E-04	7.8980E-01
81.0	8.7611E-02	2.5991E-04	7.5790E-01
82.0	8.7468E-02	2.4959E-04	7.2781E-01

83.0	8.7584E-02	2.3985E-04	6.9941E-01
84.0	8.7935E-02	2.3065E-04	6.7258E-01
85.0	8.8484E-02	2.2196E-04	6.4723E-01
86.0	8.9193E-02	2.1373E-04	6.2324E-01
87.0	9.0029E-02	2.0595E-04	6.0054E-01
88.0	9.0956E-02	1.9857E-04	5.7903E-01
89.0	9.1933E-02	1.9158E-04	5.5865E-01
90.0	9.2922E-02	1.8495E-04	5.3932E-01
91.0	9.3885E-02	1.7866E-04	5.2098E-01
92.0	9.4784E-02	1.7269E-04	5.0356E-01
93.0	9.5581E-02	1.6701E-04	4.8701E-01
94.0	9.6241E-02	1.6162E-04	4.7128E-01
95.0	9.6730E-02	1.5649E-04	4.5632E-01
96.0	9.7016E-02	1.5160E-04	4.4208E-01
97.0	9.7069E-02	1.4695E-04	4.2852E-01
98.0	9.6864E-02	1.4252E-04	4.1560E-01
99.0	9.6375E-02	1.3830E-04	4.0328E-01
100.0	9.5585E-02	1.3427E-04	3.9154E-01
101.0	9.4478E-02	1.3043E-04	3.8034E-01
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103.0	9.1267E-02	1.2326E-04	3.5943E-01
104.0	8.9157E-02	1.1992E-04	3.4968E-01
105.0	8.6711E-02	1.1672E-04	3.4035E-01
106.0	8.3935E-02	1.1366E-04	3.3144E-01
107.0	8.0845E-02	1.1074E-04	3.2291E-01
108.0	7.7460E-02	1.0794E-04	3.1475E-01
109.0	7.3798E-02	1.0526E-04	3.0694E-01
110.0	6.9890E-02	1.0269E-04	2.9946E-01
111.0	6.5772E-02	1.0024E-04	2.9229E-01
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113.0	5.7052E-02	9.5627E-05	2.7885E-01
114.0	5.2543E-02	9.3464E-05	2.7254E-01
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116.0	4.3483E-02	8.9398E-05	2.6068E-01
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122.0	2.0357E-02	7.9019E-05	2.3042E-01
123.0	1.7797E-02	7.7520E-05	2.2605E-01
124.0	1.5793E-02	7.6080E-05	2.2185E-01
125.0	1.4419E-02	7.4695E-05	2.1781E-01
126.0	1.3742E-02	7.3365E-05	2.1393E-01
127.0	1.3829E-02	7.2085E-05	2.1020E-01
128.0	1.4746E-02	7.0855E-05	2.0661E-01
129.0	1.6558E-02	6.9672E-05	2.0316E-01
130.0	1.9323E-02	6.8534E-05	1.9985E-01
131.0	2.3097E-02	6.7440E-05	1.9666E-01
132.0	2.7930E-02	6.6388E-05	1.9359E-01
133.0	3.3869E-02	6.5376E-05	1.9064E-01
134.0	4.0955E-02	6.4403E-05	1.8780E-01
135.0	4.9223E-02	6.3467E-05	1.8507E-01
136.0	5.8699E-02	6.2567E-05	1.8245E-01
137.0	6.9407E-02	6.1702E-05	1.7992E-01
138.0	8.1362E-02	6.0870E-05	1.7750E-01
139.0	9.4570E-02	6.0071E-05	1.7517E-01

140.0	1.0903E-01	5.9302E-05	1.7292E-01
141.0	1.2473E-01	5.8563E-05	1.7077E-01
142.0	1.4167E-01	5.7854E-05	1.6870E-01
143.0	1.5980E-01	5.7172E-05	1.6671E-01
144.0	1.7910E-01	5.6518E-05	1.6481E-01
145.0	1.9954E-01	5.5890E-05	1.6298E-01
146.0	2.2107E-01	5.5288E-05	1.6122E-01
147.0	2.4361E-01	5.4710E-05	1.5953E-01
148.0	2.6712E-01	5.4156E-05	1.5792E-01
149.0	2.9152E-01	5.3626E-05	1.5637E-01
150.0	3.1673E-01	5.3118E-05	1.5489E-01
151.0	3.4266E-01	5.2632E-05	1.5347E-01
152.0	3.6924E-01	5.2167E-05	1.5212E-01
153.0	3.9635E-01	5.1724E-05	1.5083E-01
154.0	4.2389E-01	5.1300E-05	1.4959E-01
155.0	4.5177E-01	5.0897E-05	1.4841E-01
156.0	4.7987E-01	5.0512E-05	1.4729E-01
157.0	5.0806E-01	5.0147E-05	1.4623E-01
158.0	5.3623E-01	4.9800E-05	1.4522E-01
159.0	5.6428E-01	4.9471E-05	1.4426E-01
160.0	5.9207E-01	4.9160E-05	1.4335E-01
161.0	6.1946E-01	4.8866E-05	1.4249E-01
162.0	6.4636E-01	4.8589E-05	1.4168E-01
163.0	6.7264E-01	4.8328E-05	1.4093E-01
164.0	6.9817E-01	4.8084E-05	1.4021E-01
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166.0	7.4651E-01	4.7645E-05	1.3893E-01
167.0	7.6911E-01	4.7448E-05	1.3836E-01
168.0	7.9049E-01	4.7267E-05	1.3783E-01
169.0	8.1057E-01	4.7101E-05	1.3735E-01
170.0	8.2927E-01	4.6950E-05	1.3691E-01
171.0	8.4647E-01	4.6814E-05	1.3651E-01
172.0	8.6208E-01	4.6693E-05	1.3616E-01
173.0	8.7606E-01	4.6587E-05	1.3585E-01
174.0	8.8833E-01	4.6494E-05	1.3558E-01
175.0	8.9879E-01	4.6416E-05	1.3535E-01
176.0	9.0741E-01	4.6353E-05	1.3516E-01
177.0	9.1420E-01	4.6303E-05	1.3502E-01
178.0	9.1907E-01	4.6268E-05	1.3492E-01
179.0	9.2195E-01	4.6247E-05	1.3486E-01
180.0	9.2290E-01	4.6240E-05	1.3484E-01