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FORMULATING ANALYTIC EXPRESSIONS FOR ATOMIC
COLLISION CROSS SECTIONS

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Formulating Analytic Expressions for Atomic Collision Cross Sections

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Methods to formulate analytic expressions for atomic collision cross sections as a function of projectile energy are described on the basis of the experiences of the data compilation work for more than 20 years. Topics considered are the choice of appropriate functional forms for the expressions and optimization of adjustable parameters. To make extrapolation possible, functions to be used should have the form with reasonable asymptotic behavior. In this respect, modified Green–McNeal formulas have been found useful for various atomic collision cross sections. For ionization processes, a modified Lotz formula has often given a good fit. The ALESQ code for least-squares fits has been convenient to optimize adjustable parameters in analytic expressions.

Keywords: Analytic Expression Atomic Collision, Cross Section, Data Compilation

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原子衝突断面積に対する解析的表式の導出法

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(2003年6月16日受理)

20 年余にわたるデータ収集の経験をふまえ、原子衝突断面積を入射粒子エネルギーの関数として解析的に表す式を導出する方法について述べる。適切な関数形の選び方と調節パラメータの最適化の問題を取り上げる。データの外挿を可能にするため、合理的な漸近形を持つ関数を使用することが重要である。この点で、修正型 Green-McNeal 公式が、各種の原子衝突断面積に対し有用であることが分かった。イオン化過程に対しては、修正型 Lotz 公式がしばしば良好な適合を示した。解析的表式中の調節パラメータの最適化には、最小二乗法のための ALESQ コードが便利であった。

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1. Introduction

Experimental data becomes more useful when they are expressed by an analytic function fitted to them. In general, there are different purposes of fitting functions to data. Here are some examples:

- (1) To determine an unknown value in a theoretical relation.
- (2) To analyze experimental data for identifying material included in a sample.
- (3) To establish a semiempirical or an empirical relation, or to give recommended values of data, for quantities obtainable only by elaborate study.

One of the present authors (T. T.) has been cooperating in the compilation of data on atomic collision cross sections (the list of the titles of related publications [1-14] are given in Appendix), and has been applying function fitting to formulate analytic expressions for those cross sections as a function of projectile energy. Such an application of function fitting corresponds to (3) above. The analytic expressions obtained represent sets of most probable values of the dependent variable (the cross section in our application) as a function of the independent variable (projectile energy in our case), and allows one to get interpolated and extrapolated values.

The storage of data in the computer memory combined with polynomial fits to the data (see for example Ref. [15]) is useful for interpolation purposes, but does not serve to extrapolation of the data (this is shown by an example in Sec. 2). On the other hand, formulation of an analytic expression for data makes extrapolation possible when an appropriate functional form is used. In applying function fitting to the compiled set of data, therefore, the choice of the functional form is important. The method of optimizing the adjustable parameters of the function is also an important problem. Though there are general textbooks for the technique of fitting functions to data (see for example Refs. [16-18]), no specific and detailed treatment useful for the application to atomic collision data is found.

In the present report, the two important problems for the formulation of analytic expressions, i.e., the choice of functional form and the optimization of parameters, are discussed on the basis of the experiences of more than 20 years. The application to atomic collision cross sections as a function of projectile energy is assumed.

2. Functional Forms for Fitting

2.1. Finding Functional Forms

When a misbehaving function is used for fitting, extrapolation even to the smallest extent fails. An example is given in Fig. 1. In this figure, the result of fit [19] by the use of Chebyshev polynomial is seen to behave badly just beyond the highest-energy data point, indicating that the polynomial fit is quite useless for extrapolation. On the other hand, the result of fit [9] by the use of Green-McNeal type function [20], which has physically reasonable asymptotic trends as described in the next subsection, allows one to extrapolate the data to higher and lower energies rather reliably. Therefore, we have to make good choice of the function in formulating analytic expression for a set of data.

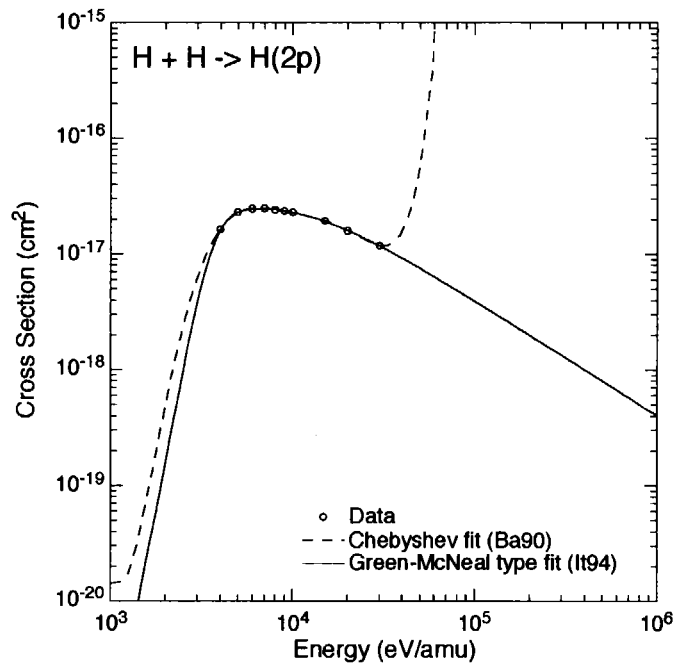


Fig. 1. Comparison of curves fitted to a set of atomic collision data (circle) by the use of Chebyshev polynomial (dashed line) and Green-McNeal type function (solid line). The Chebyshev fit uses 7 parameters [19]; The Green-McNeal type fit, 6 parameters [9].

Methods to find functional forms of analytic expressions can be classified as follows [21]:

- (1) Theoretical approach
 - derive from a simple model
 - use the prediction of an asymptotic theory
 - use a scaling law
 - replace some constants in a theoretical equation (based on a simple model) by adjustable parameters
 - replace a theoretical equation by a simple equation with similar behavior
- (2) Empirical approach
 - find a possible functional form by plotting data
- (3) Combined approach

In the actual situation of getting an analytic expression for complicated phenomenon, it is not always possible to find a good theoretical approach. However, it is desirable at least to know the asymptotic trend from theory or experimental data (examples are given in Subsecs. 2.2 and 2.4).

2.2. Charge Transfer Cross Sections

Earlier work to express atomic collision cross sections by analytic expressions was done by Green and McNeal [20] for the total cross section for electron capture by H^+ . They used the following function:

$$\sigma = \sigma_0 \frac{(Za)^\Omega (E - E_t)^\nu}{J^{\Omega+\nu} + E^{\Omega+\nu} + (Za)^\Omega E^\nu (E/C)^\Lambda}, \quad (1)$$

where σ_0 is the convenient cross section unit of $1 \times 10^{-16} \text{ cm}^2$, Z is the number of electrons in the target atom or molecule, E is projectile energy, E_t is threshold energy, and a , Ω , ν , J , C and Λ are adjustable parameters. The following nature of Green–McNeal formula provides its justification:

- (1) Low and intermediate energy region: The formula is similar to the theoretical formulas of Rapp and Francis [22].

- (2) High energy region: The formula has the asymptotic form similar to Bohr's semiclassical argument and Born's approximation.

The similarities described in (1) and (2) are discussed in Ref. [20] as follows: Rapp–Francis formula for the low-energy region behaves as Eq. (1) for small E with $\nu = 2$. The result of Rapp and Francis in the intermediate-energy region is proportional to $[\ln(E_c/E)^{1/2}]^2$ (E_c is a constant), and this can be replaced by $(E_c/E)^\Omega$ to a good approximation. At high energies, Bohr's semiclassical argument gives the dependence proportional to v^{-r} (v is the velocity of the projectile and r is a constant) with $r = 6$. On the other hand, Born's approximation gives $r = 12$ or 11. Experiment gives different values for various substances from $r = 3$ to 7.

We have used modifications of Green–McNeal formula for various charge transfer cross sections (for earlier works, see Refs. [3, 4]). The modified formula is given by

$$\sigma = \sigma_0 \{f(E_1) + a_7 f(E_1/a_8)\}, \quad (2)$$

where the function f and the argument E_1 are given by

$$f(E) = \frac{a_1 (E/E_R)^{a_2}}{1 + (E/a_3)^{a_2+a_4} + (E/a_5)^{a_2+a_6}}, \quad (3)$$

$$E_1 = E_0 - E_t, \quad (4)$$

E_R is a convenient energy to make the energy variable dimensionless [we use Rydberg energy multiplied by the ratio of the projectile mass to the electron mass (25.0 keV for atomic hydrogen)], and a_1, a_2, \dots and a_8 represent adjustable parameters. Examples of fits by Eq. (2) are shown in Figs. 2–5, which have been adapted from Ref. [8].

Figure 2 represent a fit to a narrow peak with four adjustable parameters. The function used is Eq. (2) without the second term and with Eq. (3) without the last term in the denominator, i.e.

$$\sigma = \sigma_0 \frac{a_1 (E_1/E_R)^{a_2}}{1 + (E_1/a_3)^{a_2+a_4}}. \quad (2a)$$

Figure 3 represents a fit to a broad peak with six adjustable parameters. The function used is Eq. (2) without the second term and with full terms of Eq. (3), i.e.

$$\sigma = \sigma_0 \frac{a_1 (E_1/E_R)^{a_2}}{1 + (E_1/a_3)^{a_2+a_4} + (E_1/a_5)^{a_2+a_6}}. \quad (2b)$$

Figure 4 represents a fit to a broad peak with a shoulder; and Fig. 5, a fit to a double peak. For these two fits, all the eight adjustable parameters in Eqs. (2) and (3) are used.

It is to be noted that the modified Green-McNeal formulas can also be applied to various atomic collision cross sections other than charge transfer processes. Namely, we can use Eqs. (2), (2a) and (2b) as follows:

- (1) When the cross section simply rises and decays linearly in logarithmic scales (such behavior is rather common in many atomic collision cross sections showing a narrow peak), Eq. (2a) is useful.
- (2) When the rise or the decay near the broad peak of the cross section shows an appreciable deviation from linearity (i.e. bending) in logarithmic scales, Eq. (2b) is useful, the middle term in the denominator serving as a correction for the deviation.
- (3) When the cross section shows a double peak or a shoulder beside a peak, Eq. (2) is useful, the second term serving to express the second peak or the shoulder.

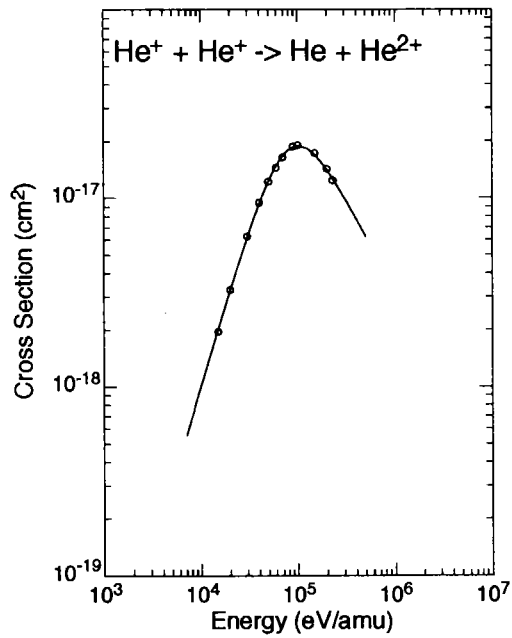


Fig. 2. A fit by Eq. (2a) to the dependence on energy of the cross section showing a narrow peak. The number of adjustable parameters used is 4. (Adapted from Ref. [8].)

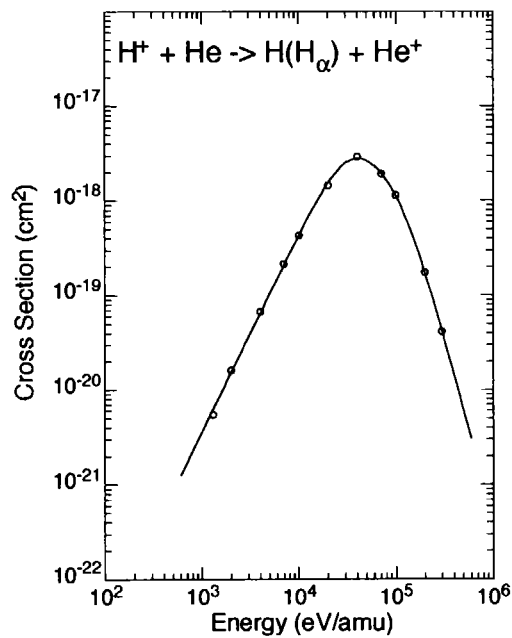


Fig. 3. A fit by Eq. (2b) to the dependence on energy of the cross section showing a broad peak. The number of adjustable parameters used is 6. (Adapted from Ref. [8].)

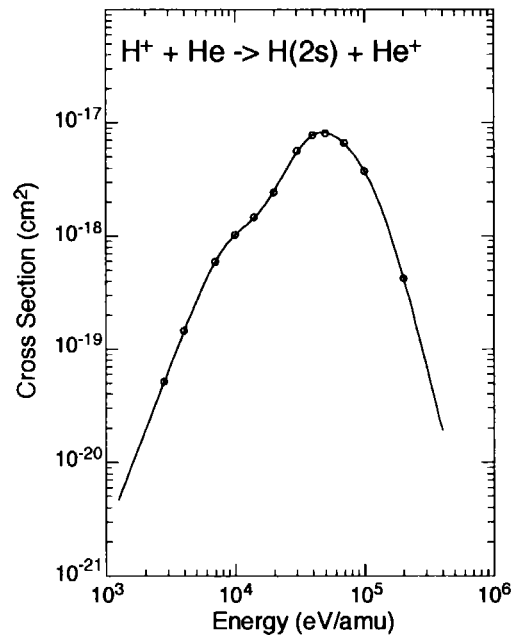


Fig. 4. A fit by Eq. (2) to the dependence on energy of the cross section showing a peak with a shoulder. The number of adjustable parameters used is 8. (Adapted from [8].)

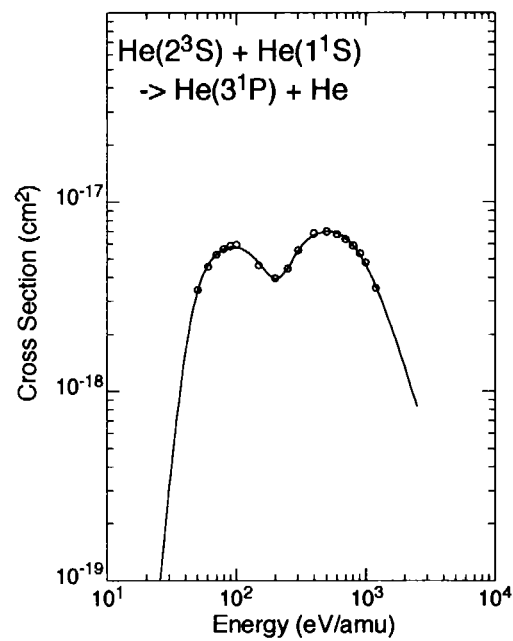


Fig. 5. A fit by Eq. (2) to the dependence on energy of the cross section showing a double peak. The number of adjustable parameters used is 8. (Adapted from [8].)

2.3. Cross Section Curves with More Structures

When dependence on energy of a cross section shows a number of peaks, it is useful to add more terms of the form of Eq. (3) to Eq. (2):

$$\sigma = \sigma_0 [f_1 + f_2 + f_3 + f_4 + \dots], \quad (2c)$$

where f_i ($i=1, 2, 3, 4, \dots$) denotes the functions of the type of Eq. (3), with or without the last term in the denominator, and with or without coefficients like a_7 and a_8 in Eq. (2). Earlier use of Eq. (2c) was made in the formulation of analytic expressions reported by Ito et al. [8-11] for collision cross sections of H, H₂, He and Li atoms and molecules.

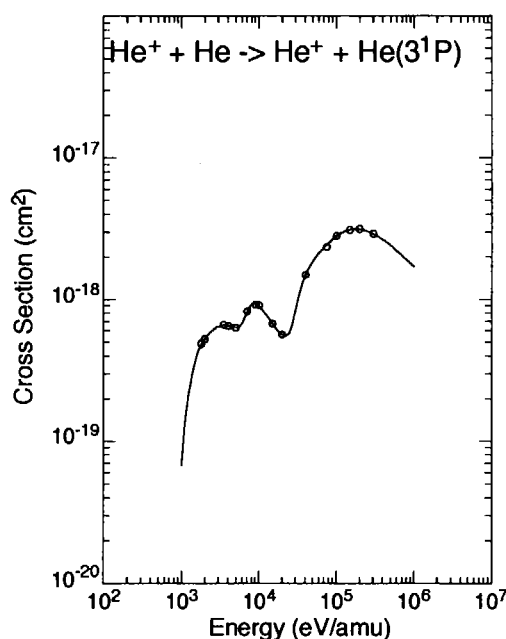


Fig. 6. A fit of Eq. (2c) (with three terms) to the dependence on energy of the cross section showing a triple peak. The number of adjustable parameters used is 11. (Adapted from Ref. [9].)

Examples of fits of Eq. (2c) to a triple and a quadruple peak are given in Figs. 6 and 7. The curve in Fig. 6 uses Eq. (2c) with three terms having a total of 11 parameters, i.e. the following functional form:

$$\sigma = \sigma_0 [f_1(E_1, a_6) + a_7 f_1(E_1/a_8, a_9) + a_{10} f_2(E_1/a_{11})], \quad (2d)$$

where the functions f_1 and f_2 are given by

$$f_1(E, \alpha) = \frac{a_1 (E/E_R)^{a_2}}{1 + (E/a_3)^{a_2+a_4} + (E/a_5)^{a_2+\alpha}} \quad (3a)$$

$$f_2(E) = \frac{a_1 (E/E_R)^{a_2}}{1 + (E/a_5)^{a_2+a_6}}. \quad (3b)$$

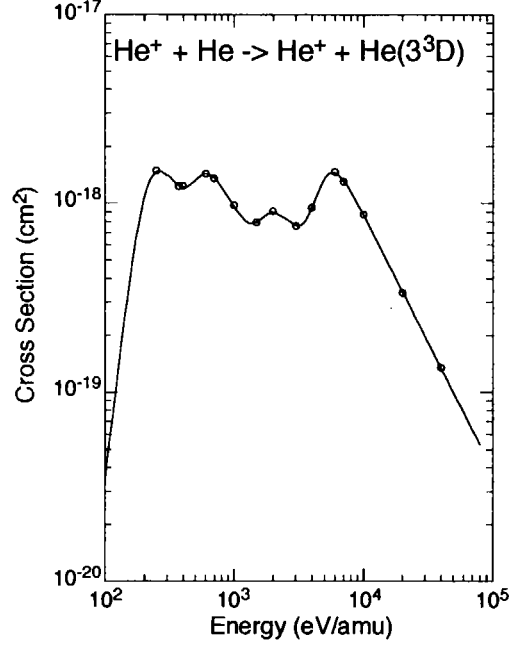


Fig. 7. A fit of Eq. (2c) (with four terms) to the dependence on energy of the cross section showing a quadruple peak. The number of adjustable parameters used is 10. (Adapted from [9].)

The third term on the right-hand side of Eq. (2d) is used for the narrowest central peak in Fig. 6. The curve in Fig. 7 uses Eq. (2c) with four terms having a total of 10 parameters [this number is less than that of Eq. (2d) for Fig. 6, because all the sub-peaks, when decomposed, simply have a form similar to Eq. (2a)]; the total functional form is given by

$$\sigma = \sigma_0 [f_3(E_1) + a_5 f_3(E_1/a_6) + a_7 f_3(E_1/a_8) + a_9 f_3(E_1/a_{10})], \quad (2e)$$

where the function f is given by

$$f_3(E) = \frac{a_1 (E/E_R)^{a_2}}{1 + (E/a_3)^{a_2+a_4}}. \quad (3c)$$

Rudd et al. [23] also used functional forms similar to Eq. (2c). They expressed cross sections of electron capture by H^+ colliding with gaseous atoms and molecules by the summation of terms like Eq. (3) over outermost subshells.

2.4. Ionization Cross Sections

For ionization cross sections, the function with the asymptotic behavior proportional to $(\ln E_0)/E_0$ as proposed by Lotz [24] is useful. For the single ionization, Lotz formula is given by

$$\sigma = a \{1 - b \exp[-c(U-1)]\} q \frac{\ln U}{E_t E_0} \quad (5)$$

where a , b and c are constants, U is given by

$$U = E_0/E_t, \quad (6)$$

q is the number of electrons in the outermost shell. The asymptotic behavior of the Lotz formula is based on the results of the theoretical calculations by Bethe [25] and Rudge and Schwartz [26].

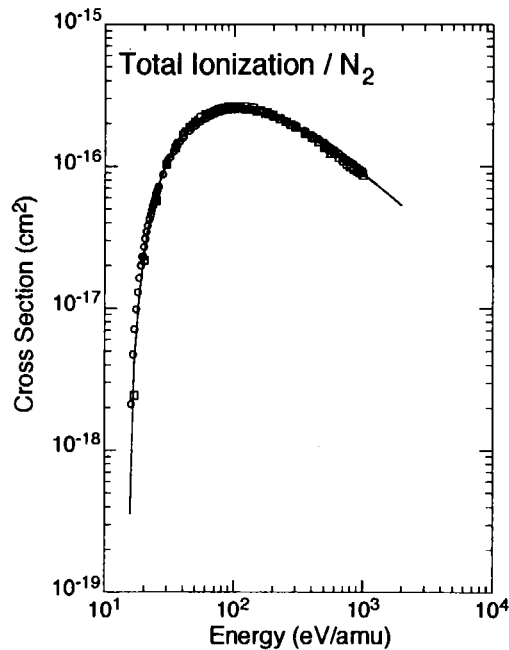


Fig. 8. A fit of Eq. (7) to the dependence on energy of the cross section of electron impact ionization of N_2 .

We have expressed the behavior near the threshold in a form different from the one in Eq. (5) and gotten a modified Lotz formula [13]:

$$\sigma = \sigma_0 a_1 [(\ln U + a_2)/E_t E_0] / [1 + (a_3/E_1)^{a_4}], \quad (7)$$

where E_1 is given by Eq. (4) on page 5. An example of fit of Eq. (7) to an ionization cross section is shown in Fig. 8. The use of the Green-McNeal type equation with the same number of parameters, i.e. Eq. (2a), gives an almost similar curve, but its root-mean square deviation from the data is a little worse than the use of Eq. (7). This indicates the excellence of the modified Lotz formula for ionization cross sections.

2.5. Other Specific Cross Sections

Olson et al. [27] used the following formula in fitting the cross section of electron removal from hydrogen atoms in collisions with positive ions:

$$\sigma/q = a(bq/E_0)[1 - \exp(-E_0/bq)]\sigma_0, \quad (8)$$

where q is the charge on the incident ion, and a and b denote adjustable parameters.

Phaneuf et al. [28] developed a formula to express general scaling relations for the charge exchange processes involving iron ions:



where M represents neutral H, H₂ or He. Their formula is given by

$$\sigma(q, E_0) = \frac{Aq \ln(B\sqrt{q}/E_0)}{1 + CE_0^2/q + D(E_0/\sqrt{q})^{4.5}}, \quad (10)$$

where A , B , C and D denote adjustable parameters.

At first glance it seems to be possible to use Eqs. (8) and (10) also for the other atomic collision cross sections that have the trend of being almost constant at low energies. To check this possibility, representative cases of these equations as given below are plotted in Fig. 9.

$$y = (1/x)[1 - \exp(-x)] \quad (8a)$$

$$y = (1/x)[1 - \exp(-x/10)] \quad (8b)$$

$$y = \ln(10^2/x) / [1 + x^2 + (x/10)^{4.5}]. \quad (10a)$$

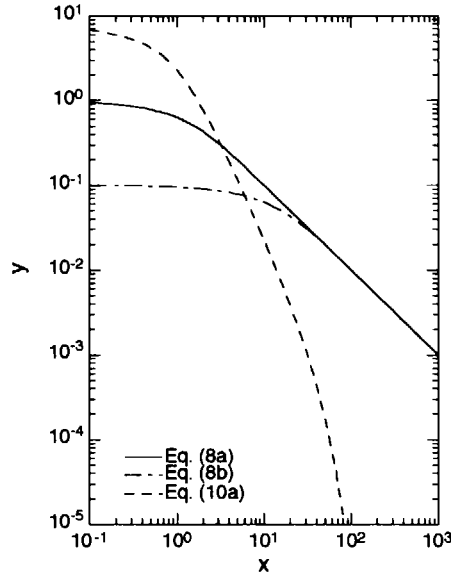


Fig. 9. Plot of representative cases of Eqs. (8) and (10), showing limitations of these equations.

Figure 9 shows that Eqs. (8) and (10) have severe limitations at high energies. Namely, Eq. (8) has the fixed asymptotic behavior proportional to $1/E_0$, and Eq. (10) has the upper bound, given by $B\sqrt{q}$, to the applicable energy region. Therefore, it is difficult to apply these equations to cross sections with various high-energy trends.

3. Optimization of Adjustable Parameters

3.1. Algorithm for Optimization

In fitting an analytic function to a set of data, it is necessary to optimize the values of adjustable parameters in the function. There are various algorithms for optimization (see for example [17]), and many program packages are commercially available. However, it is convenient to adopt such a program that can be modified easily by users according to their demand. We have been using the computer code ALESQ, which was developed by Tabata and Ito [21] for the method of least-squares fit and is written in FORTRAN. The algorithm used in ALESQ is called Levenberg–Marquardt algorithm or maximum-neighborhood algorithm (see [16]). In ALESQ a strategy developed by Tabata and Ito [29] for faster convergence is incorporated.

3.2. Weighting Data Points

Ideally data points should be weighted by:

$$w_i = \frac{N/s_i^2}{\sum_{i=1}^N (1/s_i^2)}, \quad (11)$$

where w_i is the weight for the i th data point, N is the number of data points, and s_i is the standard deviation of the i th data point. In most cases of data compilation, however, values of s_i are not available.

For the set of data that range over an order of magnitude or more, it is a good practice to assume uncertainties of approximately equal relative magnitude ($s_i = \text{const} \cdot y_i$). Then we have

$$w_i = \frac{N/y_i^2}{\sum_{i=1}^N (1/y_i^2)}. \quad (12)$$

For the set of data with large fluctuations, however, Eq.-(12) favors data points with values lower than average. To avoid this, Tabata and Ito [21] developed the method of two-step fitting, which can be described as follows:

First step: Function $\ln y$ is fitted to data $\{\ln y_i\}$ with

$$w_i = 1. \tag{13}$$

Second step: Function y_1 is fitted to data $\{y_i\}$ with

$$w_i = \frac{N/y_1^2(x_i)}{\sum_{i=1}^N [1/y_1^2(x_i)]}, \tag{14}$$

where y_1 denotes the function y with the values of the adjustable parameters obtained in the first step.

3.3. Finding Initial Values

Let us consider the example of fitting Eq. (2a) to a sample data set. The data set we use here is the cross section for C^+ production by electron collision with CO plotted in Fig. 10 (adapted from Ref. [13]).

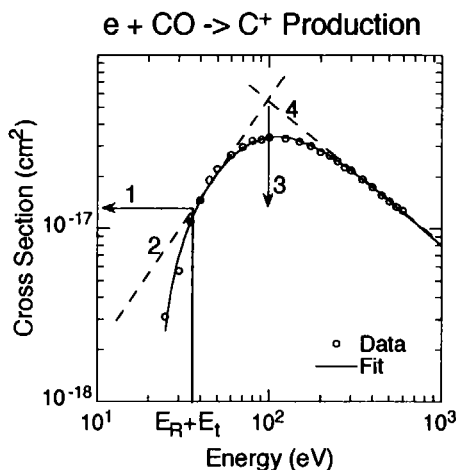


Fig. 10. Example of determining initial values of adjustable parameters for optimization. (Adapted from [13].)

We have $E_t = 2.24 \times 10^{-2}$ keV and $E_R = 1.361 \times 10^{-2}$ keV to be put in Eq. (2a). The initial values for a_1 , a_2 , a_3 and a_4 can be estimated as follows (arrows and lines referred to are those of Fig. 10):

$$a_1 = 1.3 \times 10^{-1}$$

(from the vertical scale of arrow 1, divided by 10^{-16}) (15)

$$a_2 = 1.5 \text{ (from the gradient of line 2)} \quad (16)$$

$$a_3 = 1.0 \times 10^{-1} \text{ (keV) (from the horizontal scale of arrow 3)} \quad (17)$$

$$a_4 = 1.0 \text{ (from the absolute gradient of line 4).} \quad (18)$$

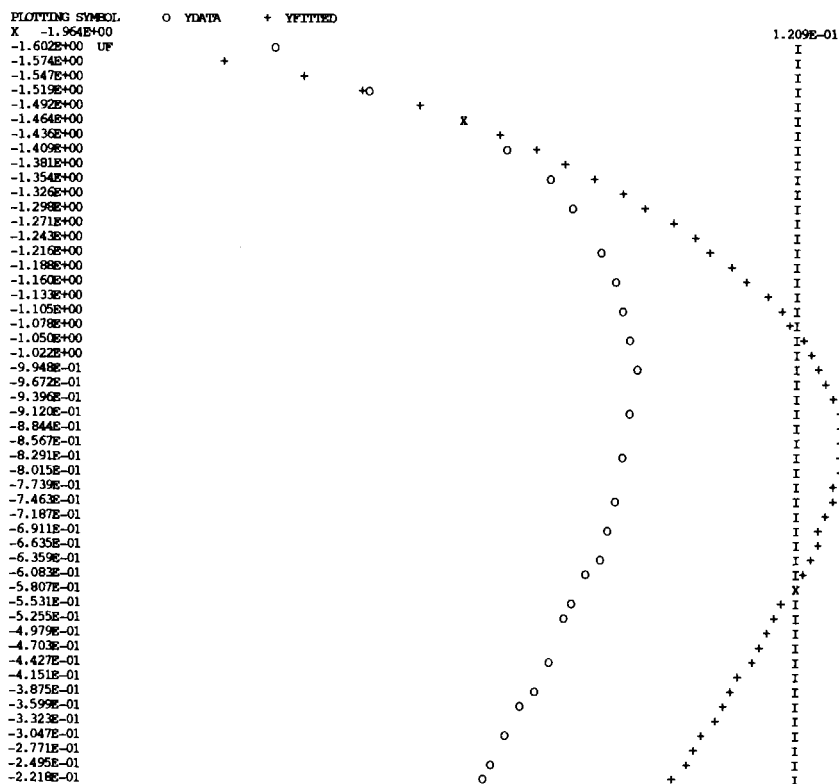


Fig. 11. Rough plot of the analytic expression (+) with initial values of adjustable parameters to compare with data (o). The symbol x is used for plotting when the symbols + and o overlap. The vertical axis represents projectile energy; and the horizontal axis, cross section. Scales are logarithmic.

With these initial values we can make a rough plot to compare the analytic expression with the data. Such a plot generated by the ALESQ code in the “check” mode is shown in Fig. 11. This figure has been produced by a simple FORTRAN subprogram included in ALESQ. The ALESQ code also gives the rms deviation of the analytic expression from the data, and it is 2.4 (240%) for the present initial values. This deviation is large. We can see from Fig. 10 that the analytic expression is larger than the data except for the lowest energies and that the maximum cross section appears at higher energy for the analytic expression than the data. Therefore, the increase of the value of a_1 and the decrease of the value of a_3 would reduce the deviation. For the simple function of Eq. (2a), however, we can start optimization from these initial values.

Optimization by ALESQ sometimes comes to a dead end for certain combinations of data and function even for considerably good initial values. In such a case, fitting a partial function to partial set of data or temporarily fixing some parameters would make progress toward the final solution. It is a good idea to use $|a_i|$ instead of a_i in the function subprogram for calculating the fitting function when a_i should be a positive definite.

3.4. Checking Results

After the computation of optimization, we should first look at the errors of the fit and the plot. These are shown in Table 1 and Fig. 12 for the example problem we are considering. If the results are not satisfying, we should change the functional form and try again.

Table 1. Part of the output list of ALESQ showing the rms relative residual, the maximum in magnitude of residual, the relative rms deviation of data from the equation and the final values and errors of adjustable parameters.

| | |
|--|-----------------------------|
| RMS RELATIVE RESIDUAL | = 5.90643E-02 |
| MAXIMUM IN MAGNITUDE OF RESIDUAL | = 2.214E-01 AT DATA NO. 2 |
| RELATIVE RMS DEVIATION OF DATA FROM EQUATION | = 5.81E-02 |
| A(1) = | 1.216085675E-01 +/- 3.5E-03 |
| A(2) = | 9.357022265E-01 +/- 3.6E-02 |
| A(3) = | 8.532963359E-02 +/- 7.3E-03 |
| A(4) = | 8.724773152E-01 +/- 5.5E-02 |

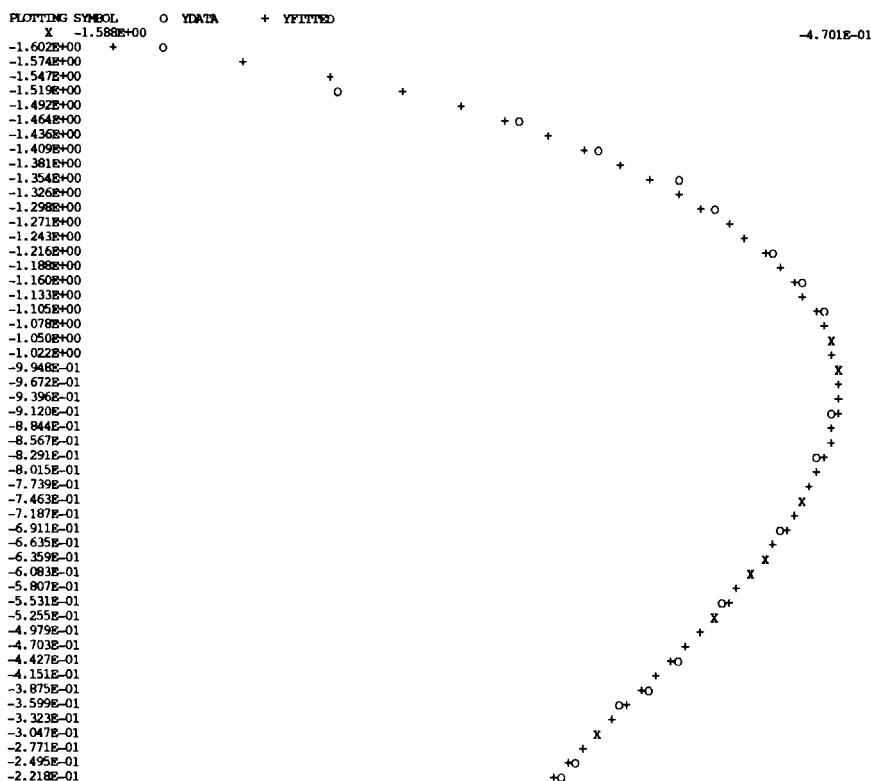


Fig. 12. Rough plot of the analytic expression (+) with the final values of adjustable parameters to compare with data (o). The symbol x is used for plotting when the symbols + and o overlap. The vertical axis represents projectile energy; and the horizontal axis, cross section. Scales are logarithmic.

3.5. Rounding Parameters

It is nonsensical to retain all the digits of the final values of the adjustable parameters given by ALESQ as shown in Table 1. We should round the parameters at the minimum necessary number of digits so as to reproduce one or two digits of the relative rms deviation δ of data from the equation (the value of δ is given in the third row of Table 1). For this purpose, it generally suffices to round each parameter at the place of the second digit of its error. In the example above, this gives: $a_1 = 1.216 \times 10^{-1}$, $a_2 = 9.36 \times 10^{-1}$, $a_3 = 8.53 \times 10^{-2}$ and $a_4 = 8.72 \times 10^{-1}$. Running ALESQ in the “check” mode with these rounded parameters, we find the corresponding value of δ to be 5.9%, satisfying our requirement.

4. Concluding Remarks

Modified Green–McNeal formulas have been useful to make analytic expressions of various atomic collision cross sections as a function of projectile energy. For ionization cross sections, a modified Lotz formula has often rendered a good fit. The ALESQ code for least-squares fit has helped us to optimize adjustable parameters in analytic expressions, though some techniques as mentioned in the last paragraph of Subsec. 3.3 are necessary for masterly use of it.

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Appendix

In this appendix the list of publications made by the JAERI group for the compilation of atomic collision cross sections are given, including one for which Shirai worked together with a group at IAEA. Among these publications, those not cited in Secs. 2 and 3 would also be useful as references for the formulation of analytic expressions.

- (1) Cross sections for charge transfer of helium atoms and ions colliding with gaseous atoms and molecules [1].
- (2) Single-electron-capture cross sections of multiply-charged ions colliding with H, H₂ and He [2].
- (3) Cross sections for charge transfer of hydrogen atoms and ions colliding with gaseous atoms and molecules [3].
- (4) Analytic cross sections for charge transfer of hydrogen atoms and ions colliding with metal vapors [4].
- (5) A semiempirical formula for single-electron-capture cross sections of multiply charged ions [5].
- (6) Partial cross-sections for single-electron capture of hydrogen ions [6].
- (7) Extended scaling of cross-sections for the ionization of H, H₂ and He by multiply charged ions [7].
- (8) Analytic cross sections for collisions of H, H₂, He and Li atoms and ions with atoms and molecules. I [8].
- (9) Analytic cross sections for collisions of H, H₂, He and Li atoms and ions with atoms and molecules. II [9].
- (10) Analytic cross sections for collisions of H, H₂, He and Li atoms and ions with atoms and molecules. III [10].
- (11) Analytic cross sections for collisions of H, H₂, He and Li atoms and ions with atoms and molecules. IV [11].
- (12) Analytic cross sections for collisions of H⁺, H²⁺, H³⁺, H, H₂, and H⁻ with hydrogen molecules [12].
- (13) Analytic cross sections for electron collisions with CO, CO₂, and H₂O relevant to edge plasma impurities [13]

- (14) Analytic cross sections for electron collisions with hydrocarbons:
 CH_4 , C_2H_6 , C_2H_4 , C_2H_2 , C_3H_8 , and C_3H_6 [14].
- (15) Recommended cross sections for state-selective electron capture in collisions of C^{6+} and O^{8+} ions with atomic hydrogen [30].

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国際単位系 (SI) と換算表

表1 SI基本単位および補助単位

| 量 | 名称 | 記号 |
|-------|--------|-----|
| 長さ | メートル | m |
| 質量 | キログラム | kg |
| 時間 | 秒 | s |
| 電流 | アンペア | A |
| 熱力学温度 | ケルビン | K |
| 物質の量 | モル | mol |
| 光度 | カンデラ | cd |
| 平面角 | ラジアン | rad |
| 立体角 | ステラジアン | sr |

表2 SIと併用される単位

| 名称 | 記号 |
|---------|-----------|
| 分, 時, 日 | min, h, d |
| 度, 分, 秒 | °, ', " |
| リットル | l, L |
| トン | t |
| 電子ボルト | eV |
| 原子質量単位 | u |

1 eV = 1.60218 × 10⁻¹⁹ J
 1 u = 1.66054 × 10⁻²⁷ kg

表5 SI接頭語

| 倍数 | 接頭語 | 記号 |
|-------------------|------|----|
| 10 ¹⁸ | エクサ | E |
| 10 ¹⁵ | ペタ | P |
| 10 ¹² | テラ | T |
| 10 ⁹ | ギガ | G |
| 10 ⁶ | メガ | M |
| 10 ³ | キロ | k |
| 10 ² | ヘクト | h |
| 10 ¹ | デカ | da |
| 10 ⁻¹ | デシ | d |
| 10 ⁻² | センチ | c |
| 10 ⁻³ | ミリ | m |
| 10 ⁻⁶ | マイクロ | μ |
| 10 ⁻⁹ | ナノ | n |
| 10 ⁻¹² | ピコ | p |
| 10 ⁻¹⁵ | フェムト | f |
| 10 ⁻¹⁸ | アト | a |

表3 固有の名称をもつ SI組立単位

| 量 | 名称 | 記号 | 他のSI単位による表現 |
|---------------|--------|----|---------------------|
| 周波数 | ヘルツ | Hz | s ⁻¹ |
| 力 | ニュートン | N | m·kg/s ² |
| 圧力, 応力 | パスカル | Pa | N/m ² |
| エネルギー, 仕事, 熱量 | ジュール | J | N·m |
| 工率, 放射束 | ワット | W | J/s |
| 電気量, 電荷 | クーロン | C | A·s |
| 電位, 電圧, 起電力 | ボルト | V | W/A |
| 静電容量 | ファラド | F | C/V |
| 電気抵抗 | オーム | Ω | V/A |
| コンダクタンス | ジーメンズ | S | A/V |
| 磁束 | ウェーバ | Wb | V·s |
| 磁束密度 | テスラ | T | Wb/m ² |
| インダクタンス | ヘンリー | H | Wb/A |
| セルシウス温度 | セルシウス度 | °C | |
| 光束 | ルーメン | lm | cd·sr |
| 照射度 | ルクス | lx | lm/m ² |
| 放射能 | ベクレル | Bq | s ⁻¹ |
| 吸収線量 | グレイ | Gy | J/kg |
| 線量当量 | シーベルト | Sv | J/kg |

表4 SIと共に暫定的に維持される単位

| 名称 | 記号 |
|----------|-----|
| オングストローム | Å |
| バ | b |
| バ | bar |
| ガ | Gal |
| キュリー | Ci |
| レントゲン | R |
| ラ | rd |
| レ | rem |

1 Å = 0.1 nm = 10⁻¹⁰ m
 1 b = 100 fm² = 10⁻²⁸ m²
 1 bar = 0.1 MPa = 10⁵ Pa
 1 Gal = 1 cm/s² = 10⁻² m/s²
 1 Ci = 3.7 × 10¹⁰ Bq
 1 R = 2.58 × 10⁻⁴ C/kg
 1 rd = 1 cGy = 10⁻² Gy
 1 rem = 1 cSv = 10⁻² Sv

(注)

- 表1-5は「国際単位系」第5版, 国際度量衡局 1985年刊行による。ただし, 1 eV および 1 uの値は CODATAの1986年推奨値によった。
- 表4には海里, ノット, アール, ヘクターも含まれているが日常の単位なのでここでは省略した。
- barは, JISでは流体の圧力を表す場合に限り表2のカテゴリに分類されている。
- EC閣僚理事会指令では bar, barnおよび「血圧の単位」mmHgを表2のカテゴリに入れていない。

換算表

| 力 | N (=10 ⁵ dyn) | kgf | lbf |
|---|--------------------------|----------|----------|
| | 1 | 0.101972 | 0.224809 |
| | 9.80665 | 1 | 2.20462 |
| | 4.44822 | 0.453592 | 1 |

粘度 1 Pa·s(N·s/m²) = 10 P(ポアズ) (g/(cm·s))
 動粘度 1 m²/s = 10⁴ St(ストークス) (cm²/s)

| 圧 | MPa (=10 bar) | kgf/cm ² | atm | mmHg (Torr) | lbf/in ² (psi) |
|---|----------------------------|----------------------------|----------------------------|---------------------------|----------------------------|
| | 1 | 10.1972 | 9.86923 | 7.50062 × 10 ³ | 145.038 |
| 力 | 0.0980665 | 1 | 0.967841 | 735.559 | 14.2233 |
| | 0.101325 | 1.03323 | 1 | 760 | 14.6959 |
| | 1.33322 × 10 ⁻⁴ | 1.35951 × 10 ⁻³ | 1.31579 × 10 ⁻³ | 1 | 1.93368 × 10 ⁻² |
| | 6.89476 × 10 ⁻³ | 7.03070 × 10 ⁻² | 6.80460 × 10 ⁻² | 51.7149 | 1 |

| エネルギー・仕事・熱量 | J (=10 ⁷ erg) | kgf·m | kW·h | cal (計量法) | Btu | ft·lbf | eV |
|-------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|----------------------------|
| | 1 | 0.101972 | 2.77778 × 10 ⁻⁷ | 0.238889 | 9.47813 × 10 ⁻⁴ | 0.737562 | 6.24150 × 10 ¹⁸ |
| | 9.80665 | 1 | 2.72407 × 10 ⁻⁶ | 2.34270 | 9.29487 × 10 ⁻³ | 7.23301 | 6.12082 × 10 ¹⁹ |
| | 3.6 × 10 ⁶ | 3.67098 × 10 ⁵ | 1 | 8.59999 × 10 ⁵ | 3412.13 | 2.65522 × 10 ⁶ | 2.24694 × 10 ²⁵ |
| | 4.18605 | 0.426858 | 1.16279 × 10 ⁻⁶ | 1 | 3.96759 × 10 ⁻³ | 3.08747 | 2.61272 × 10 ¹⁹ |
| | 1055.06 | 107.586 | 2.93072 × 10 ⁻⁴ | 252.042 | 1 | 778.172 | 6.58515 × 10 ²¹ |
| | 1.35582 | 0.138255 | 3.76616 × 10 ⁻⁷ | 0.323890 | 1.28506 × 10 ⁻³ | 1 | 8.46233 × 10 ¹⁸ |
| | 1.60218 × 10 ⁻¹⁹ | 1.63377 × 10 ⁻²⁰ | 4.45050 × 10 ⁻²⁶ | 3.82743 × 10 ⁻²⁰ | 1.51857 × 10 ⁻²² | 1.18171 × 10 ⁻¹⁹ | 1 |

1 cal = 4.18605 J (計量法)
 = 4.184 J (熱化学)
 = 4.1855 J (15 °C)
 = 4.1868 J (国際蒸気表)
 仕事率 1 PS (仏馬力)
 = 75 kgf·m/s
 = 735.499 W

| 放射能 | Bq | Ci |
|-----|------------------------|-----------------------------|
| | 1 | 2.70270 × 10 ⁻¹¹ |
| | 3.7 × 10 ¹⁰ | 1 |

| 吸収線量 | Gy | rad |
|------|------|-----|
| | 1 | 100 |
| | 0.01 | 1 |

| 照射線量 | C/kg | R |
|------|-------------------------|------|
| | 1 | 3876 |
| | 2.58 × 10 ⁻⁴ | 1 |

| 線量当量 | Sv | rem |
|------|------|-----|
| | 1 | 100 |
| | 0.01 | 1 |

