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Extrapolation of experimental data on thermonuclear reaction cross sections using the global spline method

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Abstract. *Background* Modeling processes in thermonuclear targets requires reliable data on the cross sections and rates of thermonuclear reactions. The most reliable source of such data is the regression of experimental measurements. However, existing experiments are conducted for colliding particle energies of 2–3 keV and higher, while target ignition calculations require data at energies starting from 0.1 keV. Therefore, the approximating formula must allow extrapolation to lower energies. The physical basis for such extrapolation is Gamow's formula, according to which the reaction S-factor should tend to a constant. However, the formulas for S-factors given in the literature are applicable within the corresponding experimental intervals. The question of the possibility of their downward extrapolation in energy remains open. *Purpose* In this regard, the aim of this work is to develop a new method for approximating and extrapolating experimental data on thermonuclear reaction cross sections. *Method* The method proposed in this paper is based on constructing a special type of global spline. *Results* Four reactions involving hydrogen and helium isotopes traditionally used in thermonuclear target calculations were processed. The resulting approximations are applicable in the energy range of 0.01 keV to 3.3 MeV. Their accuracy is 0.2–1%. *Conclusions* A comparison of the obtained results with the formulas most commonly used in the literature shows that the accuracy of the proposed method is 2–4 times higher than the world standard.

Key words and phrases: thermonuclear reactions, cross-sections, reactions rates, approximations

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1. Introduction

Controlled thermonuclear fusion is considered one of the most promising areas of modern energy. A large number of different reactor concepts have been proposed in the literature (see, for example, [1, 2]). Numerical modelling is the main tool used to analyse them. Theoretical calculations of controlled thermonuclear fusion targets predict ignition, but this has not been observed in experiments. Therefore, all components of simulation should be carefully analysed. Ignition conditions are sensitive to the cross-sections of thermonuclear reactions in the temperature range of 0.1–1 keV. The most reliable source of such data is the regression of experimental measurements. However, existing experiments are conducted for colliding particle energies of 2–3 keV and higher [3]. Therefore, the approximating formula must allow extrapolation to lower energies. The physical basis for such extrapolation is Gamow's formula, according to which the S-factor of a reaction should tend toward a constant.

There are dozens of experimental works on measuring cross sections containing thousands of points. A number of articles have carried out statistical processing of such experiments [4–18]. In these articles, a certain a priori dependence of the cross section on energy is selected, and the coefficients of this formula are selected. This method is quite reliable within the limits of experimental energies. The question of whether they can be extrapolated downward in energy remains open. Specialized extrapolation methods for such data have not been developed.

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We previously proposed a regularised double-period method [19], which significantly improved the accuracy of the approximation and extrapolation of cross sections and reaction rates. In the present work, an even more reliable method is constructed, based on the use of a special type of global spline. It provides extrapolation of experimental data on cross section by the Gamow's formula [20]. The accuracy achieved is 0.2–1.1%, which is 2 or more times more accurate than the world standard.

2. Method

Global spline Let us consider an array of experimental points: arguments x_i and functions $u_i \pm \delta_i$, $1 \leq i \leq I$, $I \gg 1$, where δ_i are absolute measurement errors. From the meaning of the problem, it is known that $u(x)$ is a smooth function with not too large higher derivatives, however, experimental errors δ_i can be significant.

Let us construct an approximation on the interval $[x_i, x_I]$. Let us introduce a uniform grid y_n with step h

$$y_n = (x_I - x_i) \frac{n-1}{N}, \quad 1 \leq n \leq N+1, \quad y_1 = 0, \quad y_{N+1} = x_I.$$

In general, it may be not uniform. We will consider the grid adaptation procedure further. Let us construct an approximation of the form

$$S(x) = a_0 + \sum_{n=1}^{N+1} a_n (x - y_{n-1})_+^3. \quad (1)$$

Here, a_n , $1 \leq n \leq N+1$ are the approximation coefficients. The following notation is used

$$(x - y_{n-1})_+^3 = \begin{cases} (x - y_{n-1})^3, & x > y_{n-1}, \\ 0, & x \leq y_{n-1}. \end{cases}$$

The first term is the global part of the spline, the terms under the sum are local “additions”. Thus, the approximation is continuous along with the second derivative. The coefficients a_n are determined in the standard way using the least squares method. Let us define the relative root mean square deviation per point (RMSD)

$$\Delta = \frac{1}{I - N - 2} \sum_{i=1}^I \frac{(S(x_i) - u_i)^2}{\delta_i^2}.$$

Minimising RMSD $\Delta = \min$ leads to a system of algebraic equations for the coefficients a_n

$$\sum_{n=1}^N A_{nk} a_n = B_k, \quad A_{nk} = \sum_{i=1}^I \frac{1}{\delta_i^2} \varphi_n(x_i) \varphi_k(x_i), \quad B_k = \sum_{i=1}^I \frac{1}{\delta_i^2} \varphi_k(x_i) u_i.$$

For brevity, we introduce the following notation for the basis functions

$$\phi_n(x) = \begin{cases} 1, & n = 1, \\ (x - y_{n-1})_+^3, & 2 \leq n \leq N+1. \end{cases}$$

Extrapolation Let us note one important circumstance. When extrapolating using traditional methods, the width of the confidence interval increases rapidly as we move away from the end of the experimental range. Thus, for the simplest linear extrapolation, the width of the confidence interval increases proportionally to the square of the “range” of extrapolation (i.e., the length of the segment from the end of the experimental range to the point at which the extrapolant is calculated). The proposed approach does not have this disadvantage. Since the extrapolation is performed by a constant, the width of the confidence interval for the extrapolation is constant and equal to that at the left end of the experimental range. This demonstrates the high reliability of the proposed method.

Calculation of the confidence interval In [19], a procedure for statistically reliable estimation of the accuracy of the obtained curve was developed. It begins with a comparison of the experimental points and the found mean square approximation. In fact, the data from different laboratories are compared and their original accuracy estimates are corrected.

Next, a random “playout” of points is performed. In this case, the mean is determined by the constructed approximation, and the standard deviation is equal to the experimental error. For the new set of “pseudo-experimental” points obtained, a new approximation $\lg S(\lg E)$ is constructed. This procedure is repeated a sufficient number of times. As a result, we obtain a “bundle” of approximating curves. Their standard deviation is a good estimate of the confidence interval of the initial approximation. This procedure was called the virtual experiment method.

If many experimental points are used, the width of the confidence interval turns out to be much smaller than one would expect from experiments conducted by a single laboratory. For well-studied reactions, the errors of the best of known methods are 2%.

Grid adaptation The coordinates of the spline grid nodes are internal parameters of the method. Therefore, they can be adjusted to improve the results.

- 1) By choosing the position of the leftmost node y_0 , we can increase the accuracy of the extrapolation to the left. Let us perform a series of calculations with different positions of the node y_0 . For each calculation, we will find the width of the confidence interval and choose the position y_0 at which the specified width is minimal.
- 2) For a number of reactions, the S-factor turned out to be a rapidly oscillating function. In these cases, a finer spline grid step was selected in the corresponding segments of the experimental range.

3. Reaction rates

Let there be a local thermodynamic equilibrium in the substance with a temperature T . Then the rate of the thermonuclear reaction is determined by the convolution $\sigma(E)\sqrt{(2E/M)}$ with the Maxwellian distribution

$$K(T) = \frac{\pi}{\sqrt{M}} \left(\frac{2}{\pi T} \right) \int_0^\infty \sigma(E) E \exp\left(-\frac{E}{T}\right) dE.$$

The integral was calculated numerically by high-precision quadrature with the substitution of the approximation $\sigma(E)$.

The confidence interval of the dependence $K(T)$ is also determined by the virtual experiment method. For the most studied reactions, accuracy of best of known methods is 1–4% at low temperatures and decreases significantly at high temperatures.

Reaction rate tables are inconvenient to use in gas-dynamic codes. It is desirable to replace them with approximate formulas with a small number of parameters. We constructed such formulas using the double period method [19]. The approximation in physical units is as follows

$$\lg K(T) = \sum_{k=0}^6 (\xi_k \cos kt + \eta_k \sin kt), \text{ where } t = \pi/5.3(\lg T - 0.65), \quad (2)$$

$$-2 \leq \lg T \leq 3.3.$$

Here, the temperature is taken in keV units.

4. Results

S-factors Traditionally, four key reactions are considered in calculations of controlled thermonuclear fusion



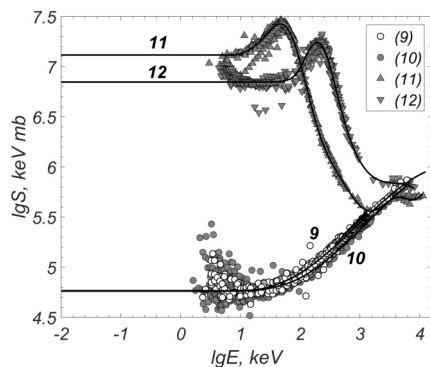


Figure 1. Approximations of the dependence of the S-factor on energy (in c.m.e.) and experimental data [3] for reactions: ○ – (3), • – (4), ▲ – (5), ▼ – (6)

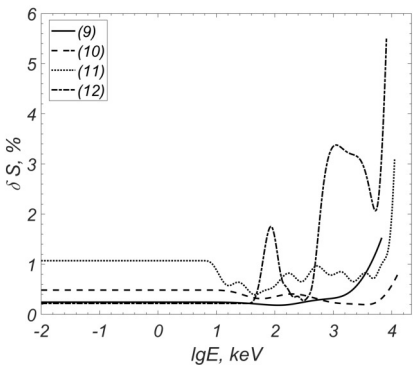


Figure 2. Dependence of S-factor errors on energy (in c.m.s.) for reactions (3)–(6)



There is a large amount of experimental data available for these reactions (~ 2000 points for all 4 reactions), collected in the EXFOR library [3]. A number of approximations have been proposed in the literature over the years. In the work [19], approximations were constructed using the regularised double period method. Their accuracy is 0.8. In Russian literature, Kozlov's formulas [18] are widely used, as well as the approximations given in the monograph [21]. Among foreign publications, the work of Bosch and Hale [12] is considered the most authoritative.

Let us process the data on reactions (3)–(6) using the proposed method. The graphs of the constructed approximations for S-factors are shown in Figure 1. The coefficients and nodes of the approximations are given in Table 1. The nature of the dependencies of reactions (3) and (4) is quite simple, so a minimum number of approximation nodes (and coefficients) was used to describe these dependencies (Tab. 1). Reactions (5) and (6) are more complex in nature, with clear resonances in the 45 and 200 keV regions, respectively. An non-uniform grid was used to accurately convey the characteristics of the curves. The number of nodes (and coefficients) reaches 9. Thus, the proposed method allows us to limit ourselves to a small number of approximation parameters. This is convenient for practical application.

Confidence intervals were calculated using the virtual experiment method. They are shown in Figure 2. It can be seen that at the left end of the experimental range, the approximation error is 0.2–1.1% at the left end. This accuracy exceeds the world level by 4 times. The accuracy of extrapolation down the energy scale is also 0.2–1.1%.

Reaction rates The approximation of reaction rates is shown in Figure 3. The approximation coefficients of the tabulated function $K(T)$ are presented in Table 2.

The use of the global spline method made it possible to increase the accuracy of the approximation to values of 0.2–1.1% in the low temperature range. This exceeds previous results several times over.

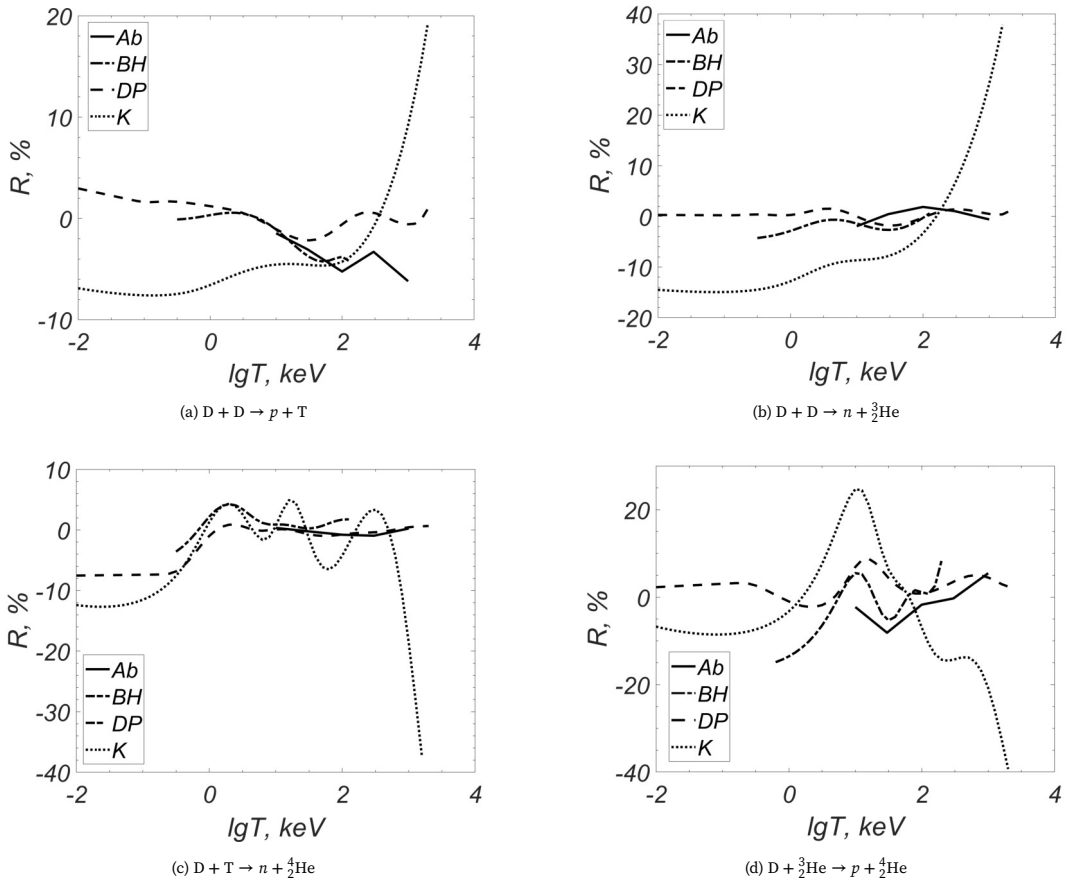


Figure 3. Comparison with other reaction rate approximation formulas: DP — double period method [19], K — Kozlov's formula [18], BH — Bosch-Hale's formula [12], Ab — Abramovich et al. formula [21]

5. Discussion

Let us compare the obtained results with known approximations for reaction cross-sections and rates. The extremely high accuracy of our approximations allows us to evaluate the accuracy of previously known results, i.e. Kozlov's formulas [18], Bosch-Hale approximations [12], Abramovich et al. approximations [21] and the regularised double-period method [19].

S-factors Figure 4 shows the relative deviation of these approximations from the proposed approximation. Each curve is given in the energy range specified in the original work. We can see that in the low energy range ($E < 100 \text{ keV}$), the error of Kozlov's formula reaches 20%. The Bosch-Hale and Abramovich et al. formulas have an accuracy of $\sim 10\text{--}15\%$. The regularised double-period method provides an accuracy of 1.5–3.5%.

Reactivities Figure 3 shows the relative deviation of known formulas for reaction rates from the curves presented in this work. Kozlov's formulas [18] have an error of $\sim 7\text{--}15\%$ at temperatures $T \sim 10 \text{ eV}$. The Bosch-Hale's formulas [12] provide an accuracy of no worse than 5% across the entire temperature range for reactions (3)–(5). For reaction (6), the accuracy is slightly worse and amounts

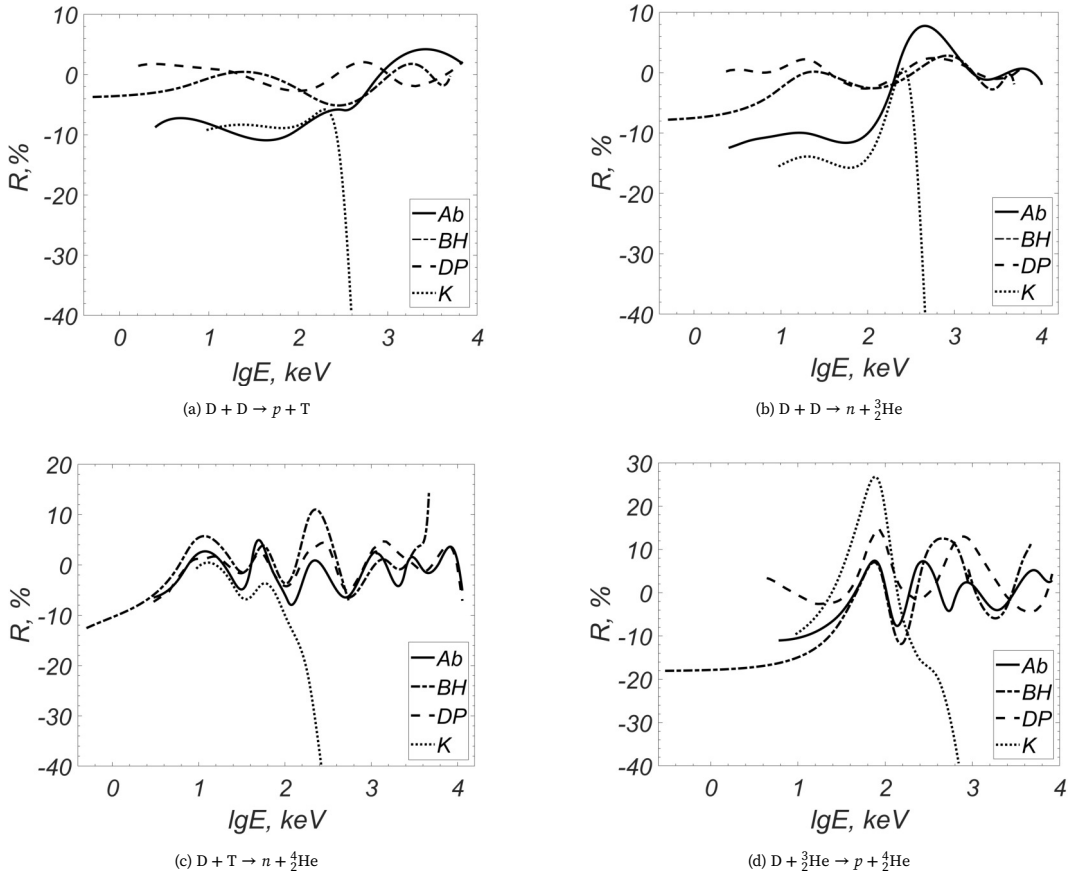


Figure 4. Comparison with other S-factor approximation formulas: DP — double period method [19], K — Kozlov's formula [18], BH — Bosch–Hale's formula [12], Ab — Abramovich et al. formula [21].

to $\sim 10\%$. The results presented in the monograph by Abramovich et al. [21] have an accuracy of no worse than 10%, but the data on the rates are presented for each reaction only for 4 points lying in the region of fairly high temperatures. The regularised double period method gives an accuracy of 1–3%.

6. Conclusion

A new method for extrapolating the energy dependence of thermonuclear reaction cross sections is proposed, based on the global spline method. The extrapolation is physically justified by the Gamow model, according to which the reaction S-factor tends to a constant at low energies.

The achieved accuracy of 0.2–1.1% for the cross-section and rate dependencies of thermonuclear reactions at low temperatures and energies can significantly improve the accuracy of thermonuclear target calculations in practice. Comparison with known sources indicates that the global spline method exceeds the world standard in accuracy by a factor of 3–4 or more.

Author Contributions: Development and original draft preparation, A. Belov; writing—original draft preparation, O. Topor; manuscript review and editing, Z. Dombrovskaya, L. Borodachev; writing—review and numerical experiments, O. Topor. All authors have read and agreed to the published version of the manuscript.

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Table 1

Values of nodes and approximation coefficients of the S-factor for reactions (3)–(6) used in Eq. (1)

	D + D → p + T		D + D → n + ³ ₂ He		D + T → n + ⁴ ₂ He		D + ³ ₂ He → p + ⁴ ₂ He	
	y _n	a _n	y _n	a _n	y _n	a _n	y _n	a _n
1	0.7085	4.7622	0.8679	4.7665	0.7761	7.1165	1.4417	6.8466
2	2.0262	0.0608	1.3027	0.1642	0.9243	1.3221	1.7351	0.4836
3	3.8428	-0.1314	2.2375	-0.1821	1.3726	-1.2944	1.9527	3.3702
4					1.8208	-3.7872	2.1704	-12.5360
5					2.2690	8.8008	2.3881	2.9941
6					2.7162	-6.7776	2.6058	16.4896
7					3.1635	3.2060	2.8235	-8.3064
8					3.6107	-4.1709	3.9159	-3.4866
9					4.0579	6.3330		

Table 2

Values of reaction rate approximation coefficients for reactions (3)–(6) used in Eq. (2)

	D + D → p + T	D + D → n + ³ ₂ He	D + T → n + ⁴ ₂ He	D + ³ ₂ He → p + ⁴ ₂ He
ξ ₀	-44.6779	-42.9257	-46.5783	-40.6976
ξ ₁	35.0087	31.8969	40.6813	17.2096
η ₁	24.3312	24.4850	23.3644	43.9668
ξ ₂	-12.7575	-10.5047	-15.4974	10.0461
η ₂	-17.0121	-17.1958	-15.3945	-32.5929
ξ ₃	4.1990	2.9014	5.9911	-11.3493
η ₃	7.6000	7.7764	6.0411	16.6916
ξ ₄	-1.2006	-0.6518	-2.1194	6.0740
η ₄	-2.5648	-2.6752	-1.2985	-6.6748
ξ ₅	0.2616	0.1025	0.5944	-2.1239
η ₅	0.5982	0.6421	0.0603	1.9900
ξ ₆	-0.0318	-0.0096	-0.1203	0.3707
η ₆	-0.0736	-0.0831	0.0822	-0.3894
Δ, %	0.5193	0.3391	0.0249	0.1233

Data Availability Statement: The source data used in this study are openly available in the EXFOR database of the International Atomic Energy Agency and original scientific works . All numerical results obtained during processing are presented in the tables and graphs of the article; additional derived data can be provided by the authors upon reasonable request.

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Declaration on Generative AI: The author has not employed any generative AI tools.

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Экстраполяция экспериментальных данных по сечениям термоядерных реакций методом глобального сплайна

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Аннотация. *Предпосылки* Для моделирования процессов в термоядерных мишенях требуются достоверные данные по сечениям и скоростям термоядерных реакций. Наиболее надёжным источником таких данных является регрессия экспериментальных измерений. Однако существующие эксперименты проводятся для энергий сталкивающихся частиц 2–3 кэВ и более, в то время как для расчётов зажигания мишеней требуются данные при энергиях от 0,1 кэВ. Поэтому аппроксимирующая формула должна допускать экстраполяцию в сторону меньших энергий. Физическим основанием такой экстраполяции является формула Гамова, согласно которой S-фактор реакции должен стремиться к константе. Однако приведённые в литературе формулы для S-факторов применимы в пределах соответствующих экспериментальных отрезков. Вопрос о возможности их экстраполяции вниз по энергии остается открытым. *Цель* В связи этим, целью данной работы является разработка нового метода аппроксимации и экстраполяции экспериментальных данных по сечениям термоядерных реакций. *Метод* Предложенный в данной работе метод основан на построении глобального сплайна специального вида. *Результаты* Проведена обработка четырёх реакции с участием изотопов водорода и гелия, традиционно используемых в расчетах термоядерных мишеней. Построенные аппроксимации применимы в диапазоне 0,01 кэВ – 3,3 МэВ. Их точность составляет 0,2–1%. *Выводы* Сравнение полученных результатов с наиболее употребительными в литературе формулами показывает, что точность предложенного метода в 2–4 раза превосходит мировой уровень.

Ключевые слова: термоядерные реакции, сечения, скорости реакций, аппроксимации