

Regularization of the Double Period Method for Experimental Data Processing

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Abstract—In physical and technical applications, an important task is to process experimental curves measured with large errors. Such problems are solved by applying regularization methods, in which success depends on the mathematician's intuition. We propose an approximation based on the double period method developed for smooth nonperiodic functions. Tikhonov's stabilizer with a squared second derivative is used for regularization. As a result, the spurious oscillations are suppressed and the shape of an experimental curve is accurately represented. This approach offers a universal strategy for solving a broad class of problems. The method is illustrated by approximating cross sections of nuclear reactions important for controlled thermonuclear fusion. Tables recommended as reference data are obtained. These results are used to calculate the reaction rates, which are approximated in a way convenient for gasdynamic codes. These approximations are superior to previously known formulas in the covered temperature range and accuracy.

Keywords: experimental data processing, rates of nuclear reactions, double period method, regularization.

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1. PROBLEM

Important physical experiments are sometimes performed beyond the capabilities of experimental equipment. Systematic and random errors can be so large that the collection of experimental points produced by different authors looks like a cloud spreading around some curve. A typical example is presented in Fig. 1, which shows the cross section of the nuclear reaction $D + D \rightarrow p + T$ as a function of energy in specific coordinates. The data obtained by the various authors differ as much as sixfold! However, this is a major reaction in controlled thermonuclear fusion, so such curves have to be processed.

Usually, physicists follow two approaches. Firstly, relying on the physical interpretation of the problem, they choose specific variables in which the curve would have the simplest shape. Secondly, they try to approximate the curve by an analytical dependence with only a few fitting parameters. The values of these parameters are determined by the least squares method. Success in this approach depends on how well the approximating formula is guessed.

If the fitting parameters are much fewer than the number of experimental points and an acceptable approximation accuracy is reached, then the approximating formula can be viewed as successful. Especially valuable are formulas reproducing well-known physical dependences. In this case, we can hope for an approximation by a few parameters. However, such formulas are rarely proposed. If an approximation requires parameters that are comparable in number with the experimental points, then the form of the formula is regarded as unsuccessful and the approximation will hardly be reliable. Moreover, its extrapolation beyond the original interval can lead to large errors.

In our approach [1], instead of choosing an approximating formula, we represent the solution in the form of a specific trigonometric series, i.e., the double period method is used. To avoid spurious oscillations caused by large errors in experimental points, the method is supplemented with Tikhonov's regularizer involving only a squared second derivative. This approach is rather simple and yields nice curves admitting extrapolation beyond the original interval. It can be used as a reliable tool when attempts to construct a good physically interpretable approximating formula fail.

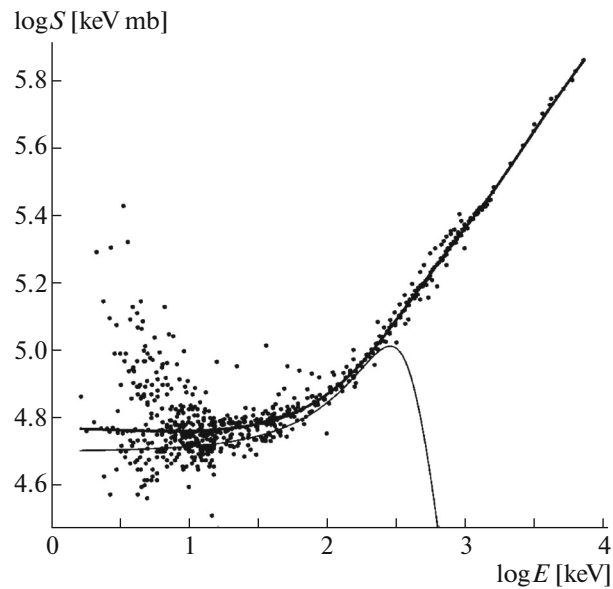


Fig. 1. S -factors for the reaction $D + D \rightarrow p + T$: the experimental values are depicted by dots, the data from Table 2, by the thick curve; and Kozlov's formula, by the thin curve.

The method is illustrated as applied to four major nuclear reactions used to compute controlled thermonuclear fusion.

2. REGULARIZATION OF THE DOUBLE PERIOD METHOD

2.1. Double Period Method

Suppose that we are given a large 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. According to the problem, $u(x)$ is a smooth function with not very large highest derivatives, but the measurement errors δ_i can be large.

To approximate smooth nonperiodic functions by Fourier series, it is convenient to use the double period method (see [2, 3]). For notational simplicity, a linear transformation is applied to the argument x , so that $\min x_i = -\pi/2$ and $\max x_i = \pi/2$. On the interval $[-\pi/2, \pi/2]$, we consider the zero Fourier harmonic and N pairs of sine-cosine harmonics. They are supplemented with M harmonics of doubled period $[-\pi, \pi]$ that are not included in the fundamental period. These harmonics are added not in sine-cosine pairs, but rather individually, so that their number M can be of any parity.

The function $u(x)$ is approximated by a sum of harmonics of the fundamental and double periods. For uniformity, we use the notation

$$u(x) \approx \sum_{n=0}^{2N+M} a_n \varphi_n(x). \quad (1)$$

The coefficients a_n are chosen so as to obtain the best approximation of $u(x)$ in the L_2 norm.

Here, the fundamental-period harmonics have indices $0 \leq n \leq 2N$ and are written as

$$\begin{aligned} \varphi_n(x) &= \cos 2mx, & \varphi'_n(x) &= -2m\varphi_{n-1}(x), & \varphi''_n(x) &= -4m^2\varphi_n(x) & \text{if } n = 2m; \\ \varphi_n(x) &= \sin 2mx, & \varphi'_n(x) &= 2m\varphi_{n+1}(x), & \varphi''_n(x) &= -4m^2\varphi_n(x) & \text{if } n = 2m - 1. \end{aligned} \quad (2)$$

Formulas (2) involve the derivatives of these harmonics, which will be used later. The double-period harmonics have indices $2N + 1 \leq n \leq 2N + M$ (i.e., they are written so that they follow the fundamental-period harmonics) and have the form

$$\begin{aligned}\varphi_n(x) &= \cos(2m - 1)x, & \varphi'_n(x) &= -(2m - 1)\varphi_{n-1}(x), \\ \varphi''_n(x) &= -(2m - 1)^2\varphi_n(x) & \text{if } n &= 2N + 2m; \\ \varphi_n(x) &= \sin(2m - 1)x, & \varphi'_n(x) &= (2m - 1)\varphi_{n+1}(x), \\ \varphi''_n(x) &= -(2m - 1)^2\varphi_n(x) & \text{if } n &= 2N + 2m - 1.\end{aligned}\tag{3}$$

Formally, the fundamental-period harmonics are sufficient for the approximation as $N \rightarrow \infty$. Therefore, the terms with $n > 2N$ are redundant in this case. For finite N , sum (1) is not redundant. It was shown in [2] that adding double-period harmonics is equivalent to increasing the smoothness of the periodic extension of $u(x)$ to $[-\pi, \pi]$. Specifically, every extra double-period harmonic added increases the smoothness of $u(x)$ by 1.

For larger M , the expansions in terms of fundamental-period harmonics converge more quickly. For a fixed M , as $N \rightarrow \infty$, expression (1) approximates $u(x)$ and its q th derivatives in the C norm with $O(N^{q-M})$ accuracy. In numerical computations, only small values of M should be used, since the conditioning of the computations degrades catastrophically with increasing M . However, the values of N can be taken large to obtain a good approximation accuracy. Of course, the total number of parameters must satisfy $2N + M + 1 < I$.

2.2. Choosing a Regularizer

The method described above was developed for functions of continuous argument or functions given on a uniform grid when the values of $u(x)$ are calculated with high accuracy. In experiments, the grid x_i is highly nonuniform and can contain gaps, while the errors δ_i are frequently large. By gaps, we mean rather long segments of the argument on which there are no experimental points. Such data have to be approximated by applying regularization. A natural strategy is to use Tikhonov's stabilizer [4] involving integrals of squared derivatives of $u(x)$. Let us discuss which derivatives are reasonable to use.

Obviously, $u(x)$ and $u'(x)$ have to be approximated with good accuracy. Therefore, they cannot be involved in the stabilizer: this would lead to a decrease in their values and, accordingly, to a deterioration of the approximation. However, except for radio engineering problems, physical curves are usually fairly smooth and free of high-frequency oscillations, so that their curvature is not very large. Therefore, it is reasonable to bound $u''(x)$ by including it in the stabilizer. This is usually sufficient for the spurious oscillations to be effectively suppressed, so that there is no need to include higher order derivatives in the stabilizer.

Another practical advantage of including the second derivative is that the double differentiation of a sine or cosine yields a function of the same type, which simplifies the algorithm.

There are two circumstances to be taken into account regarding the particular problem of approximating nuclear reaction cross sections. First, an important point is the relative (rather than absolute) accuracy of cross section approximations, since the cross sections have a wide range of values. Second, specific variables are chosen so that $u(x) \approx \text{const}$ for the smallest x_i . Therefore, the values of $(u')^2$ and $(u'')^2$ with large weighting factors have to be added to the stabilizer on the left boundary to ensure that the fitted curve becomes a horizontal line. With these considerations taken into account, the least squares method yields the formulation

$$\sum_{i=1}^I \left(\frac{u(x_i) - u_i}{\delta_i} \right)^2 + \alpha \int_{-\pi/2}^{\pi/2} [u''(x)]^2 dx + \beta [u'(-\pi/2)]^2 + \gamma [u''(-\pi/2)]^2 = \min,\tag{4}$$

where $\alpha, \beta, \gamma > 0$. Substituting (4) into (1), we obtain the minimization problem for the coefficients a_n .

It is reasonable to evaluate the integral in (4) in the sense of functions of continuous argument without using the grid x_i . In doing this, we need to remember that each of the subsystems (2) and (3) is orthogonal,

but they are not orthogonal to each other, although the sines of one subsystem are orthogonal to the cosines of the other.

Remark 1. A traditional approach to regularization is that minimization problem (4) is reduced to a differential equation for $u(x)$. The order of this equation is twice as high as the order of the maximum derivative included in the regularizer. This equation requires additional boundary conditions, whose number is equal to the order of the equation. A formal statement of such conditions usually leads to a regularized solution differing noticeably from the true one near the boundaries of the interval.

In addition, solving a boundary value problem for a high-order differential equation is a task of certain mathematical difficulty. For this reason, high-order regularizers are rarely used in practice.

This difficulty can be naturally overcome by applying the double period method. Specifically, a high-order regularizer can easily be used in this method without applying lowest order derivatives. Moreover, the proximity of a regularized solution to the exact one is much easier to achieve, while the solution algorithm does not become more complicated.

Remark 2. Tikhonov's integral stabilizer ensures that the whole regularized curve overall behaves nicely. Accordingly, it is reasonable to apply it to a broad class of real-world problems. The specific features of the given problem (data processing in a thermonuclear experiment) are reflected by the additional terms associated with boundary conditions. For many other problems, they are not required. In that case, all formulas presented below can be used with $\beta = \gamma = 0$.

2.3. Linear System

The minimization in (4) with respect to a_n yields a system of linear equations for determining these coefficients. To write it, we introduce some auxiliary notation. Specifically, the following scalar products are associated with the experimental material:

$$\begin{aligned} \langle \varphi_n, \varphi_k \rangle = \langle \varphi_k, \varphi_n \rangle &= \sum_{i=1}^I \frac{\varphi_n(x_i)\varphi_k(x_i)}{\delta_i^2}, \quad 0 \leq n, \quad k \leq 2N + M; \\ \langle \varphi_n, u \rangle &= \sum_{i=1}^I \frac{\varphi_n(x_i)u_i}{\delta_i^2}, \quad 0 \leq n \leq 2N + M. \end{aligned} \quad (5)$$

In the case of arbitrary nodes and weights (which corresponds to an actual experimental material), all these matrix elements are nonzero, i.e., the matrix of the linear system is dense.

We also introduce scalar products of basis functions associated with the regularizer. These scalar products have a block matrix containing two square diagonal blocks:

$$(\varphi_0, \varphi_0) = \pi, \quad (\varphi_n, \varphi_k) = \frac{\pi}{2} \delta_{n,k} \quad \text{for } 0 < n, \quad k \leq 2N \quad \text{or} \quad 2N + 1 \leq n, \quad k \leq 2N + M. \quad (6)$$

It also involves two rectangular nondiagonal blocks, in which the elements corresponding to the scalar products of a sine from one subsystem by a cosine from the other are equal to zero. These zero elements are located in a staggered manner. Therefore, for $n \leq 2N$ and $k \geq 2N + 1$, we can write

$$(\varphi_n, \varphi_k) = \begin{cases} 0 & \text{if } n+k \text{ is odd;} \\ \frac{(-1)^{(m-n)/2}}{n-m+1} - \frac{(-1)^{(m+n)/2}}{n+m+1}, \quad m = k - 2N & \text{if } n \text{ and } k \text{ are odd;} \\ \frac{(-1)^{(m-n)/2}}{n-m+1} - \frac{(-1)^{(m+n)/2}}{n+m-1}, \quad m = k - 2N & \text{if } n \text{ and } k \text{ are even.} \end{cases} \quad (7)$$

The second nondiagonal block with $k \leq 2N$ and $n \geq 2N + 1$ is symmetric to the given one. Additionally, we introduce the harmonic frequencies

$$\begin{aligned} \omega_n &= n + \frac{1 - (-1)^n}{2} = 2 \left[\frac{n+1}{2} \right], \quad 0 \leq n \leq 2N; \\ \omega_n &= m - \frac{1 + (-1)^m}{2} = 2 \left[\frac{m+1}{2} \right], \quad m = n - 2N, \quad 2N + 1 \leq n \leq 2N + M. \end{aligned} \quad (8)$$

Here, the square brackets denote the integer part of a number.

With the use of this notation, the linear system becomes

$$\sum_{k=0}^{2N+M} A_{nk} a_k = \langle u, \varphi_n \rangle, \quad 0 \leq n \leq 2N + M, \quad (9)$$

where

$$A_{n,k} = \langle \varphi_n, \varphi_k \rangle + \alpha \omega_n^2 \omega_k^2 (\varphi_n, \varphi_k) + \beta \omega_n \omega_k B_{nk} + \gamma \omega_n^2 \omega_k^2 C_{n,k}; \quad (10)$$

$$B_{nk} = \begin{cases} -(-1)^{(n+k)/2} & \text{if } n \text{ and } k \text{ are odd and } 0 \leq n, k \leq 2N, \\ (-1)^{(n+k)/2} & \text{if } n \text{ and } k \text{ are even and } 2N+1 \leq n, k \leq 2N+M, \\ 0, & \text{otherwise;} \end{cases} \quad (11)$$

$$C_{nk} = \begin{cases} (-1)^{(n+k)/2} & \text{if } n \text{ and } k \text{ are even and } 0 \leq n, k \leq 2N, \\ -(-1)^{(n+k)/2} & \text{if } n \text{ and } k \text{ are odd and } 2N+1 \leq n, k \leq 2N+M, \\ 0, & \text{otherwise.} \end{cases} \quad (12)$$

2.4. Solution of the Linear System

In the approximation of functions defined with the same accuracy on a uniform grid, the scalar products $\langle \varphi_n, \varphi_k \rangle$ have a structure resembling that of the matrix (φ_n, φ_k) . It also contains two diagonal and two nondiagonal blocks. Moreover, the diagonal blocks are diagonal submatrices. This improves conditioning, so we can use even $M \sim 5-6$. However, if the grid x_i is nonuniform and δ_i are not identical, the diagonal blocks are dense and the condition number degrades substantially. In this case, the computations have to be restricted to $M = 3$, which is equivalent to the smoothness of the periodic extension of $u''(x)$. A smaller value of M does not ensure the required smoothness.

According to the properties of the least squares method, the matrix A is symmetric and positive definite. It is reasonable to solve it by Gaussian elimination without pivoting, since the pivot element is automatically on the main diagonal. This algorithm is robust even for matrices A with a rather large condition number κ (up to $\kappa \sim 10^8$ for 64-bit computations).

3. EXPERIMENTAL DATA

3.1. Measurements

Consider four major reactions used in the computation of controlled thermonuclear fusion:



Most of the available experimental data concerning their cross sections can be found in [5]. This database relies on 90 original works and contains 2000 experimental points. Data produced by different authors sometimes do not match well and can differ by 6 times! The author's error estimates are sometimes unreliable, and the approximation result depends rather strongly on δ_i .

For this reason, we performed our own critical analysis of the experiments and derived estimates for δ_i . Specifically, measurements on targets consisting of heavy metals saturated with deuterium were assigned large errors. In heavy metals, the incident beam loses much energy, and the actual energy at the moment of particle collision cannot be estimated accurately. Targets consisting of pure deuterium or its compounds with lightest elements (LiD, CD₂, CD₄, D₂O) were treated as the best. The international reputation of a laboratory and the year of performing measurements were also taken into account (for example, the Los Alamos data obtained even in 1950 were regarded as more reliable than the latest measurements con-

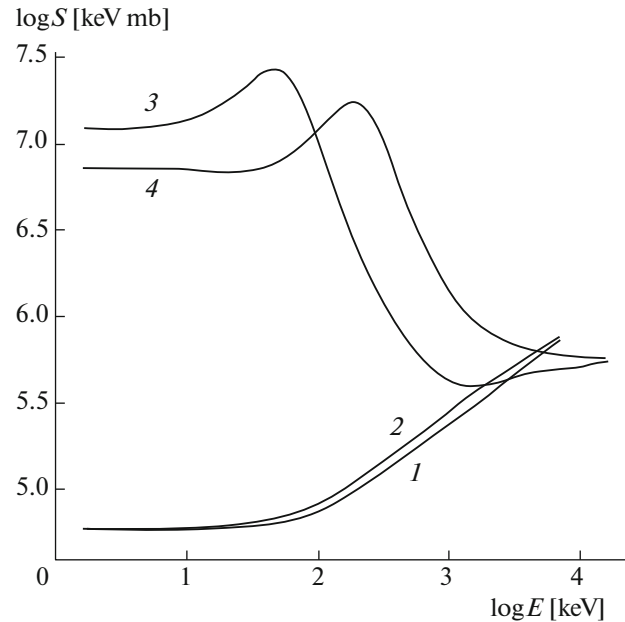


Fig. 2. S -factors from Table 2: (1) $D + D \rightarrow p + T$, (2) $D + D \rightarrow n + {}^3\text{He}$, (3) $D + T \rightarrow n + {}^4\text{He}$, and (4) $D + {}^3\text{He} \rightarrow p + {}^4\text{He}$.

ducted in some European laboratories). A detailed analysis of each work is not presented here, since this is of interest only to physicists specializing in the given area.

3.2. Variables

Let us describe how we chose variables. As an argument, it is convenient to use $x = \log E$, where E is the energy of colliding particles in the center-of-mass system. However, the reaction cross section $\sigma(E)$ or its logarithm is inconvenient when used as functions. A much more convenient variable to use is the S -factor. It is obtained by multiplying the cross section by the Gamow factor, which takes into account the probability of overcoming the Coulomb barrier:

$$S(E) = \sigma(E)E \exp\left\{\pi z_1 z_2 \sqrt{\frac{2m}{E}}\right\}, \quad (17)$$

where m is the reduced mass and z_1 and z_2 are the charges of the particles (in atomic units). The function is defined as $u = \log S$. Its value varies only by 1.5–2 units.

The resulting S -factors after processing are presented in Fig. 2. It can be seen that they are similar for both channels of the reaction $D + D$ and look like the transition from a horizontal line to a sloping one. However, for the other two reactions, they represent a curve with a maximum. These differences are associated with the substantially different physical mechanisms of the reactions. In the traditional physical approach, its own approximating formula has to be chosen for each reaction, which is rather difficult. The double period method allows us to process all these reactions in a unified manner.

4. NUMERICAL RESULTS

In all computations, we used $M = 3$. The values of N and the regularization parameters were chosen for each reaction separately taking into account the number of experimental points and their errors. More specifically, the regularization parameters were selected in the standard manner so that the difference between the regularized curve and the experiments was within the experimental errors and the curve did not contain visually noticeable oscillations. The parameters chosen for the various reactions and the approximation errors Δ in percent are given in Table 1.

Table 1. Regularization parameters in problem (4) for reactions (13)–(16)

Parameter	DD \rightarrow pT	DD \rightarrow n ³ He	DT \rightarrow n ⁴ He	D ³ He \rightarrow p ⁴ He
I	717	364	370	544
N	123	123	73	98
α	0.2	0.3	0.04	0.2
β	2000	2000	2000	2000
γ	2000	2000	2000	2000
$\Delta, \%$	1.5	1.5	2	4

Table 2. Reaction S -factors $\log S$ [keV mb]

$\log E$ [keV]	DD \rightarrow pT	DD \rightarrow n ³ He	DD \rightarrow n ⁴ He	D ³ He \rightarrow p ⁴ He	$\log E$ [keV]	DD \rightarrow pT	DD \rightarrow n ³ He	DD \rightarrow n ⁴ He	D ³ He \rightarrow p ⁴ He
0.2	4.774	4.773	7.086	6.852	2.3	4.998	5.053	6.395	7.231
0.3	4.773	4.773	7.086	6.852	2.4	5.048	5.106	6.226	7.161
0.4	4.771	4.773	7.086	6.852	2.5	5.102	5.160	6.082	7.004
0.5	4.770	4.772	7.086	6.852	2.6	5.157	5.215	5.954	6.803
0.6	4.769	4.769	7.090	6.852	2.7	5.212	5.272	5.844	6.610
0.7	4.768	4.767	7.098	6.852	2.8	5.267	5.330	5.754	6.435
0.8	4.768	4.768	7.108	6.851	2.9	5.321	5.389	5.684	6.283
0.9	4.767	4.772	7.120	6.848	3.0	5.373	5.448	5.635	6.156
1.0	4.768	4.776	7.137	6.844	3.1	5.426	5.504	5.605	6.052
1.1	4.770	4.781	7.161	6.840	3.2	5.481	5.557	5.596	5.970
1.2	4.773	4.786	7.196	6.836	3.3	5.540	5.607	5.605	5.908
1.3	4.776	4.794	7.241	6.835	3.4	5.600	5.658	5.627	5.863
1.4	4.781	4.803	7.297	6.836	3.5	5.661	5.708	5.652	5.832
1.5	4.789	4.812	7.360	6.842	3.6	5.721	5.758	5.672	5.810
1.6	4.799	4.824	7.414	6.859	3.7	5.779	5.808	5.684	5.795
1.7	4.813	4.841	7.428	6.892	3.8	5.836	5.856	5.691	5.784
1.8	4.830	4.862	7.368	6.940	3.9	5.896	5.906	5.698	5.776
1.9	4.853	4.887	7.227	7.003	4.0	5.958	5.955	5.707	5.770
2.0	4.880	4.919	7.029	7.076	4.1	6.020	6.005	5.720	5.765
2.1	4.913	4.958	6.807	7.153	4.2	6.082	6.054	5.735	5.760
2.2	4.952	5.003	6.590	7.216					

It can be seen that the total number of free parameters is less than I by a factor of 1.5 to 3 depending on the reaction. Thus, high-frequency harmonics were used for the approximation, thereby ensuring good accuracy. Simultaneously, the high-frequency harmonics were well smoothed by regularization, so that the fitted curves were smooth. The numbers of harmonics were taken with a margin. Indeed, good accuracy is achieved for $N \sim 20$ and even for $N \sim 10$. Therefore, the large values of N in Table 1 are overcautious, although the amount of computations is insignificant even in this case. All the computations are easy to execute even on a 64-bit laptop.

The results were found to be rather sensitive to the value of α . Its optimal value is small. According to the interpretation of the problem, the parameters β and γ have to be rather large, which was confirmed by the computations. However, the sensitivity of the results to their choice was much lower.

Let us describe the final results. Table 2 and Fig. 2 present $\log S$ [keV mb] as a function of $\log E$ [keV] for all four reactions. Toward lower energies, each column of the table is extended as a constant. Figure 2 clearly shows that the fitted curve for each reaction has a natural shape and does not contain spurious

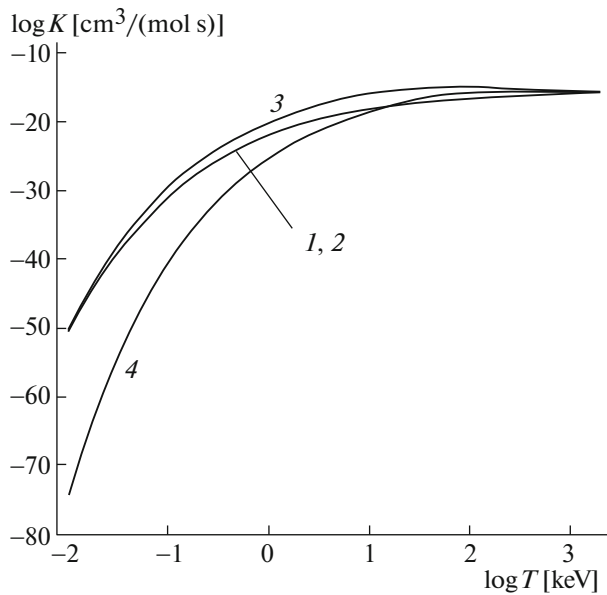


Fig. 3. Reaction rates from Table 3: (1) $D + D \rightarrow p + T$, (2) $D + D \rightarrow n + {}^3\text{He}$, (3) $D + T \rightarrow n + {}^4\text{He}$, and (4) $D + {}^3\text{He} \rightarrow p + {}^4\text{He}$.

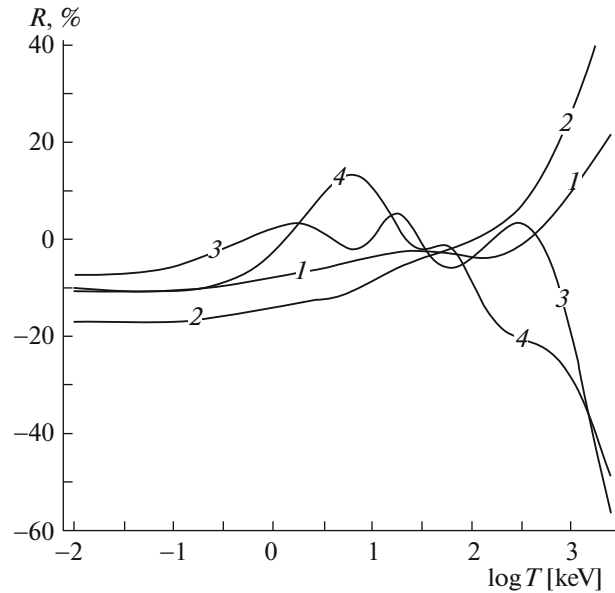


Fig. 4. Ratios of Kozlov's formulas for $K(T)$ to the data from Table 3: (1) $D + D \rightarrow p + T$, (2) $D + D \rightarrow n + {}^3\text{He}$, (3) $D + T \rightarrow n + {}^4\text{He}$, and (4) $D + {}^3\text{He} \rightarrow p + {}^4\text{He}$.

oscillations, despite the use of high-frequency harmonics. Note that, for reaction (16), there were no experimental data in the range $3 \leq \log Et \leq 3.2$. Nevertheless, the fitted curve passes this segment without exhibiting oscillations. This suggests that the proposed regularization procedure is of high quality. It can be concluded that the given method provides a reliable tool for drawing a curve through gaps in experimental data.

In practice, thermonuclear targets are rather frequently computed using Kozlov's formulas [6]. For reaction (13), this formula is presented in Fig. 1. It can be seen that, for $\log E \leq 2.45$, it agrees well with the experiments and our curve, but its accuracy quickly degrades at high energies. For the other reactions, the situation is similar. Therefore, the results in Table 2 can be used as reference data. They are more accurate than their counterparts proposed earlier (the gain in accuracy is especially large at high energies).

5. RATES OF THERMONUCLEAR REACTIONS

5.1. Tables of Rates

Suppose that a substance is in a local thermodynamic equilibrium at temperature T . Then the rate of a thermonuclear reaction is determined by the convolution of $\sigma(E)\sqrt{\frac{2E}{m}}$ with the Maxwellian distribution:

$$K(T) = \frac{\pi}{\sqrt{m}} \left(\frac{2}{\pi T} \right)^{3/2} \int_0^{\infty} \sigma(E) E \exp\left\{-\frac{E}{T}\right\} dE. \quad (18)$$

The integral is numerically evaluated using high-accuracy quadrature rules with the substitution of Fourier approximation (1).

The numerical results are given in Fig. 3 and Table 3, which present $\log K(T)$ [$\text{cm}^3/(\text{mol s})$] as a function of $\log T$ [keV]. Approximations for $K(T)$ can also be found in [6]. The deviations R of those quantities from our data in percent are shown in Fig. 4. It can be seen that, at low temperatures, R is at most 11% for reactions (13) and (16), only 5–7% for (15), and reaches 20% for (14). These improvements are

Table 3. Reaction rates $\log K(T)$ [$\text{cm}^3/(\text{mol s})$]

$\log T$, keV	DD \rightarrow pT	DD \rightarrow n ³ He	DT \rightarrow n ⁴ He	D ³ He \rightarrow p ⁴ He	$\log T$, keV	DD \rightarrow pT	DD \rightarrow n ³ He	DT \rightarrow n ⁴ He	D ³ He \rightarrow p ⁴ He
-2.0	-50.402	-50.402	-50.492	-74.292	0.8	-18.749	-18.729	-16.525	-19.629
-1.9	-47.667	-47.668	-47.582	-69.633	0.9	-18.482	-18.460	-16.217	-19.120
-1.8	-45.139	-45.140	-44.891	-65.324	1.0	-18.237	-18.213	-15.947	-18.644
-1.7	-42.803	-42.804	-42.405	-61.338	1.1	-18.013	-17.987	-15.716	-18.199
-1.6	-40.645	-40.645	-40.107	-57.651	1.2	-17.807	-17.779	-15.523	-17.784
-1.5	-38.650	-38.651	-37.984	-54.241	1.3	-17.618	-17.587	-15.369	-17.401
-1.4	-36.808	-36.809	-36.022	-51.089	1.4	-17.444	-17.410	-15.249	-17.050
-1.3	-35.107	-35.108	-34.210	-48.174	1.5	-17.283	-17.246	-15.162	-16.736
-1.2	-33.537	-33.538	-32.537	-45.479	1.6	-17.134	-17.093	-15.103	-16.462
-1.1	-32.087	-32.088	-30.993	-42.989	1.7	-16.996	-16.952	-15.069	-16.228
-1.0	-30.750	-30.750	-29.567	-40.687	1.8	-16.867	-16.820	-15.057	-16.036
-0.9	-29.517	-29.517	-28.252	-38.560	1.9	-16.747	-16.697	-15.062	-15.881
-0.8	-28.379	-28.379	-27.039	-36.596	2.0	-16.635	-16.582	-15.082	-15.762
-0.7	-27.331	-27.330	-25.920	-34.781	2.1	-16.531	-16.476	-15.114	-15.674
-0.6	-26.366	-26.365	-24.888	-33.105	2.2	-16.435	-16.377	-15.156	-15.613
-0.5	-25.476	-25.475	-23.936	-31.559	2.3	-16.345	-16.286	-15.206	-15.575
-0.4	-24.657	-24.657	-23.058	-30.131	2.4	-16.263	-16.201	-15.261	-15.556
-0.3	-23.904	-23.903	-22.248	-28.815	2.5	-16.188	-16.124	-15.318	-15.552
-0.2	-23.211	-23.210	-21.501	-27.602	2.6	-16.118	-16.052	-15.378	-15.561
-0.1	-22.573	-22.572	-20.812	-26.484	2.7	-16.054	-15.987	-15.436	-15.579
0.0	-21.988	-21.985	-20.177	-25.454	2.8	-15.995	-15.928	-15.492	-15.603
0.1	-21.450	-21.445	-19.590	-24.505	2.9	-15.940	-15.875	-15.543	-15.632
0.2	-20.957	-20.950	-19.047	-23.630	3.0	-15.888	-15.826	-15.589	-15.662
0.3	-20.504	-20.495	-18.544	-22.824	3.1	-15.841	-15.783	-15.629	-15.694
0.4	-20.089	-20.077	-18.077	-22.081	3.2	-15.796	-15.744	-15.663	-15.724
0.5	-19.708	-19.695	-17.643	-21.396	3.3	-15.755	-15.709	-15.692	-15.754
0.6	-19.360	-19.344	-17.240	-20.762	3.4	-15.716	-15.677	-15.717	-15.781
0.7	-19.041	-19.023	-16.866	-20.175					

important for physical applications. Of course, for $T > 100$ keV, Kozlov's formulas quickly become inaccurate.

Thus, the above results can be used to improve the accuracy of computing thermonuclear targets in which relatively low temperatures are primarily required. Accordingly, Table 3 can also be recommended for using as reference data. Since quadrature (18) was calculated to high accuracy, the error in these data is determined by the error of the original cross sections in Table 2. It can roughly be estimated as ± 0.007 – 0.008 for both channels of the reaction $D + D$ (which corresponds to 1.5%), as ± 0.01 for the reaction $D + T$ (i.e., 2%), and as ± 0.017 for $D + {}^3\text{He}$ (i.e., 4%).

5.2. Gasdynamic Applications

Tables of reaction rates are inconvenient for using in gasdynamic codes. It is desirable to replace them by approximating formulas with a few parameters. Such formulas were derived by applying the double period method, but without regularization, since this time we approximated a smooth mathematical curve rather than experimental points with a large scatter. The same accuracy as in Table 3 was achieved for $M = 5$ and $N = 3$.

Table 4. Coefficients of the approximation of $\log K(T)$ by a Fourier series

	DD \rightarrow pT	DD \rightarrow n ³ He	DT \rightarrow n ⁴ He	D ³ He \rightarrow p ⁴ He
ξ_0	-41.898	-42.145	-42.559	-60.504
ξ_1	30.017	30.484	33.312	53.039
η_1	24.313	24.459	24.394	43.244
ξ_2	-9.150	-9.451	-9.876	-16.233
η_2	-16.995	-17.170	-16.909	-31.497
ξ_3	2.140	2.265	2.501	3.980
η_3	7.572	7.744	7.406	15.707
ξ_4	-0.316	-0.346	-0.414	-0.749
η_4	-2.540	-2.655	-2.148	-6.055
η_5	0.580	0.630	0.411	1.734
ξ_6	0.012	0.015	0	0.004
η_6	-0.068	-0.079	0	-0.319
$\Delta, \%$	1	0.5	2.5	0.9

The number of fundamental-period harmonics turned out to be nearly the same as the number of double-period harmonics. Therefore, formula (1), in which the double-period functions follow the fundamental-period ones, is not very convenient. It is much more beneficial to write the result as a truncated Fourier series on $[-\pi, \pi]$. Then the double-period functions become odd harmonics, while the fundamental-period functions become even harmonics. The final approximation in physical units without reducing the argument to the standard interval $[-\pi/2, \pi/2]$ has the form

$$\log K(T) = \sum_{k=0}^6 (\xi_k \cos kt + \eta_k \sin kt), \quad t = \frac{\pi}{5.30} (\log T - 3.65), \quad 1.0 \leq \log T \leq 6.3. \quad (19)$$

Here, the temperature is measured in electronvolts. For all four reactions, $\eta_0 = 0$ and $\xi_5 = 0$. The other coefficients are presented in Table 4, which also lists the relative approximation errors Δ (%) in the C norm. It can be seen that the mathematical accuracy of the approximation roughly agrees with the estimated physical accuracy, so that M and N were chosen reasonably. For all reactions, the condition number of the linear system was $\kappa = 4 \times 10^6$, which is rather high, but quite acceptable for 64-bit computations.

Table 4 can be recommended for using in applied computations. Since the double period method allows reasonable extrapolation beyond the fundamental period, formula (19) can be used even in the range $0.5 \leq \log T \leq 6.8$ (in eV).

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REFERENCES

1. A. A. Belov and N. N. Kalitkin, "Processing of experimental curves by applying a regularized double period method," *Dokl. Math.* **94** (2), 602–606 (2016).
2. N. N. Kalitkin and L. V. Kuz'mina, "Approximation and extrapolation of tabulated functions," *Dokl. Math.* **62** (2), 306–310 (2000).
3. N. N. Kalitkin and K. I. Lutskii, "Optimal parameters of the double period method," *Mat. Model.* **19** (1), 57–68 (2007).
4. A. N. Tikhonov and V. Ya. Arsenin, *Solutions of Ill-Posed Problems* (Halsted, New York, 1977; Nauka, Moscow, 1979).
5. NEA Data Bank—Nuclear Data Services. <http://www.oecd-nea.org/janisweb/search/exfor>.
6. B. N. Kozlov, "Rates of thermonuclear reactions," *At. Energ.* **12** (3), 238–240 (1962).

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