https://doi.org/10.31489/2024M1/128-139 *Research article*

Isomorphism Theorems of a Series Sum and the Improper Integral

V.P. Malyshev[1], S.Sh. Kazhikenova[2], A.M. Makasheva[1,*], A.Sh. Kazhikenova[3]

[1] *Abishev Chemical and Metallurgical Institute, Karaganda, Kazakhstan;*
[2] *Abylkas Saginov Karaganda Technical University, Karaganda, Kazakhstan;*
[3] *Karaganda Buketov University, Karaganda, Kazakhstan*
(E-mail: eia_hmi@mail.ru, sauleshka555@mail.ru, astra_mun@mail.ru, aigul-kazhikenova@mail.ru)

The discrete and continuous dependencies' relationship question has been investigated. An algorithm for determining the final and total series sums through the equivalence ratio of the series common term a_n and the a_n-model function improper integral mean value within the change unit interval based on the extended integral Cauchy convergence criterion has been developed. Examples of determining for the statistical sum in the Boltzmann distribution, for the first time directly expressed through a_n-model function. This eliminates the need for calculations to accumulate the sum of the series up to a value that is specified by a certain accuracy of this sum. In addition, it allows in this case to vary the energy variation interval with any given accuracy. The conducted studies allow solving both theoretical and practical problems of physics and materials science, directly using the Boltzmann distribution (energy spectrum) to calculate the entropy, which determines the loss of thermal energy in technological processes.

Keywords: isomorphism, series sum, improper integral, Boltzmann distribution, equivalence relation.

2020 Mathematics Subject Classification: 40-02, 40C10, 44A20.

Introduction

The natural sciences are dominated by discrete (nanoparticles, atoms, molecules, genes, etc.), but continuous (electromagnetic fields, wave theory, etc.) quantities are also used to describe real processes. Classical mathematics is built on the continuity and a function limit concepts, which are difficult to apply in practice. The basis of specific calculations are the laws of discrete mathematics, which has developed as a result of only mathematical constructions recognition from a finite number of procedures and finite objects. Evolution models are continuous and discrete dynamical systems. Continuous dynamical systems are described by ordinary differential equations systems or in partial derivatives, discrete dynamical systems are described by difference equations systems. There is a certain relationship between continuous and discrete systems, regardless of the application. It is interesting to compare the continuous model properties and their discrete counterparts. And the functional dependence question arises, when it is possible to carry out the transition from continuous to discrete values and vice [1–3]. As it is known, the discrete dependencies' identification with continuous ones as the argument tends to an infinitely small value dx is the differential and integral calculus. But the relationship between discrete and continuous distributions can turn out to be definite and productive for fixed variation intervals, x, if we applied to them the isomorphism general provisions — one mathematics development the new directions [4]. Prior to this, such a relationship manifested itself when establishing the convergence of a series, i.e. sums of discrete quantities, using the Cauchy, Maclaurin series convergence integral criterion [5], according to which the series $\sum_{n=1}^{\infty} a_n$ converges if for the function $f(x)$, which takes the values a_n at the points n, namely, for $f(n) = a_n$, and for condition of monotone decrease of $f(x)$ in the region $x \geq n_0$ with observance of the inequality $f(x) \geq 0$, the convergence of the improper integral $\int_{n_0}^{\infty} f(x)dx$ is ensured. The integral Cauchy criterion greatly facilitates the series convergence

*Corresponding author. *E-mail: astra_mun@mail.ru*
Received: 11 August 2023; *Accepted:* 17 October 2023.

study, since to reduce this issue to finding out the integral convergence of a well-chosen corresponding function $f(x)$, which is easily done using the integral calculus methods. Thus, this sign establishes a certain equivalence of discrete and a variable continuous distribution. Detailed calculations, but without observing the isomorphism conditions, were presented earlier by the authors [6–10].

It is necessary to verify the proposed version provability for the series sum and the improper integral of the auxiliary a_n-model function isomorphism, the existence of which is entirely determined by the structure and form of the common term of the series and corresponds to its direct purpose for determining its sum. In this regard, the a_n-model function has a peculiarity, the similarity of which has not been found in the literature [11–17]. This originality emphasizes the insufficiency of the integral criterion for the convergence of the series and the improper Cauchy and Maclaurin integral to determine the sum of the series, copying according to the form the series common term. Such insufficiency is a consequence of using only the inequalities of a series sum and the improper integral to prove the series convergence or divergence in terms these integral the convergence or divergence. To determine of a series sum itself, an analytical, quantitative expression of its relationship with the improper integral is required for a given restriction of this relationship. In addition, isomorphism is generally aimed at introducing analytical proofs of mathematical objects similarity instead of their qualitative similarity indications. At the very least, it is not yet possible to determine a series sum based on the area inequalities formed using a_n and $f_n(x)$.

1 Determination of the equivalence relation based on the Boltzmann distribution

The Boltzmann distribution for a monatomic ideal gas in a discrete version is expressed as

$$P_i = \frac{N_i}{N} = e^{-\frac{\varepsilon_i}{kT}} / \sum_{i=1}^{\infty} e^{-\frac{\varepsilon_i}{kT}}, \tag{1}$$

where P_i is the particles fraction with the i-th energy level ε_i, and the first energy level for physical and thermodynamic reasons is equal to zero as the lowest energy value to which the equilibrium system tends. It, like quantum orbitals, is also the most populated, which is mathematically achieved by the value $exp(-\varepsilon_i/kT) = 1$ and following from (1) at $\varepsilon_i = (i-1)\triangle\varepsilon$ by the condition $P_{i+1} \leq P_i$, if $T \geq 0$, and $P_{i+1} = P_i$ at $T \to \infty$.

The series sum $\sum_{i=1}^{\infty} e^{-\frac{\varepsilon_i}{kT}}$ until recently had no limit direct expression and was estimated either from specific spectral distributions or as a continuous function

$$\int_0^{\infty} e^{-\frac{\varepsilon}{kT}} d\varepsilon = -kT \left| e^{-\frac{\varepsilon}{kT}} \right|_0^{\infty} = kT. \tag{2}$$

This result raises questions, first of all, due to its explicit energy dimension, J·particle^{-1}, which belongs not to the function, but to the argument. The function is a continuous sum of populations of infinitesimally different energy levels, and the function must be dimensionless. We will try to solve this question further as a special case of a more general solution. Meanwhile, it is possible to fairly strictly determine of the series sum (statistical sum) using the equivalence relation A, for which the series common term must be expressed in more detail and in the accepted notation

$$a_n = e^{-\frac{(n-1)\triangle\varepsilon}{kT}}, \tag{3}$$

which provide the condition: at $n = 1$ $a_1 = 1,\ \varepsilon = 0$. In this case, $\triangle\varepsilon$ is the energy variation step and kT are constants (isothermal energy distribution is considered). a_n-model function (3) is expressed as

$$f_n(x) = e^{-\frac{(x-1)\triangle\varepsilon}{kT}}, \tag{4}$$

and its improper integral (4) as

$$\int_0^\infty e^{-\frac{(x-1)\triangle\varepsilon}{kT}}dx = -\frac{kT}{\triangle\varepsilon}\left|e^{-\frac{(x-1)\triangle\varepsilon}{kT}}\right|_0^\infty = \frac{kT}{\triangle\varepsilon}e^{\frac{\triangle\varepsilon}{kT}}. \quad (5)$$

The integral (5) does not contain $x = n$ that is, it converges, and hence the series $\sum_{n=1}^{\infty} a_n$ converges according to the integral criterion for the Cauchy and Maclaurin series convergence.

If we consider the integrand (2) as a_n-model for the series $\sum_0^\infty e^{-\frac{n\triangle\varepsilon}{kT}}$, then its improper integral is expressed as

$$\int_0^\infty e^{-\frac{x\triangle\varepsilon}{kT}}dx = -\frac{kT}{\triangle\varepsilon}\left|e^{-\frac{x\triangle\varepsilon}{kT}}\right|_0^\infty = \frac{kT}{\triangle\varepsilon}. \quad (6)$$

This dimensionless result (6) can be numerically equal to kT only at $\triangle\varepsilon = 1$ J·particle^{-1}. This interval is quite acceptable, as well as any others that do not have a fundamental physical justification. It is much more convincing to use $\triangle\varepsilon = kT$. But let us continue the isomorphism possibility analysis on the chosen example in the most general form.

To determine the equivalence relation, it is required to check its independence from n in an arbitrary unit interval

$$A_1 = \frac{\int_{x=n-1}^{x=n} e^{-\frac{(x-1)\triangle\varepsilon}{kT}}dx}{e^{-\frac{(n-1)\triangle\varepsilon}{kT}}} = \frac{-\frac{kT}{\triangle\varepsilon}\left|e^{-\frac{(x-1)\triangle\varepsilon}{kT}}\right|_{x=n-1}^{x=n}}{e^{-\frac{(n-1)\triangle\varepsilon}{kT}}} = \frac{-\frac{kT}{\triangle\varepsilon}(e^{-\frac{(n-1)\triangle\varepsilon}{kT}} - e^{-\frac{(n-2)\triangle\varepsilon}{kT}})}{e^{-\frac{(n-1)\triangle\varepsilon}{kT}}} = \frac{kT}{\triangle\varepsilon}(e^{\frac{\triangle\varepsilon}{kT}} - 1) \neq f_n(n). \quad (7)$$

The equivalence relation does not depend on n, so it is possible to use formula (7) to find the series sum. But first need to make sure that get the same result for the first unit interval, $0 \div 1$:

$$A_1 = \frac{\int_0^1 f_n(x)dx}{a_n} = \frac{-\frac{kT}{\triangle\varepsilon}(1 - e^{\frac{\triangle\varepsilon}{kT}})}{1} = \frac{kT}{\triangle\varepsilon}(e^{\frac{\triangle\varepsilon}{kT}} - 1).$$

Then, according to (5) and (7), we establish an isomorphism and find the partition function in the direct calculation formula form [6], which can be used to directly calculate the series sum

$$\Sigma_{n=1}^{\infty} a_n \cong \frac{1}{A}\int_0^\infty f_n(x)dx/\Sigma_{n=1}^{\infty}e^{-\frac{(n-1)\triangle\varepsilon}{kT}} = \frac{\frac{kT}{\triangle\varepsilon}e^{\frac{\triangle\varepsilon}{kT}}}{\frac{kT}{\triangle\varepsilon}(e^{\frac{\triangle\varepsilon}{kT}} - 1)} = \frac{e^{\frac{\triangle\varepsilon}{kT}}}{e^{\frac{\triangle\varepsilon}{kT}} - 1} = \frac{1}{1 - e^{-\frac{\triangle\varepsilon}{kT}}}. \quad (8)$$

Using (8), we obtain the Boltzmann distribution calculation formula (1) with the usual indexing $i = n$

$$P_i = \frac{N_i}{N} = e^{-\frac{(i-1)\triangle\varepsilon}{kT}}/\Sigma_{i=1}^{\infty}e^{-\frac{(i-1)\triangle\varepsilon}{kT}} = e^{-\frac{(i-1)\triangle\varepsilon}{kT}} \Big/ \frac{e^{\frac{\triangle\varepsilon}{kT}}}{e^{\frac{\triangle\varepsilon}{kT}} - 1} = e^{-\frac{i\triangle\varepsilon}{kT}}(e^{\frac{\triangle\varepsilon}{kT}} - 1). \quad (9)$$

So, the entropy calculations have been dramatically simplified and become more accurate and variable [8–10]. The results of the calculation statistical sum members according to the formula (3), their sum accumulation for comparison with the calculation data according to the formula for the sum direct expression (8) are shown in Table. And Boltzmann distribution results in the form (9) to control $P_i \to 0$ and the sum convergence P_i to unity. Arbitrary $1000K$ temperature values and energy variation step $\triangle\varepsilon = \frac{1000k}{2} = 6,9032 \cdot 10^{-21}$ J·particle^{-1} were chosen for calculation.

Direct calculation by (8) gives the value $\Sigma_{i=1}^{\infty} = 2.5415$, from which the stepwise summation result is only 0.0001 less. The accuracy of calculating the statistical sum, and indeed any convergent series, can be determined or specified if the direct expression of this sum through the equivalence relation A is known, since it is possible to select any interval of the sum in a commensurate set of its members.

In this case, as in the general case, it is of great importance to set the exact limits of the discrete and integral sums in order to avoid discontinuities in the continuous summation by at least one unit interval. The fact is that the series is given by the common term number inclusive that is, by the interval from $(n-1)$ to n.

Therefore, to cover the area $a_n \times 1$, we need to start integrating from a value equal to $n-1$, and end with the series higher term number, $m > n$. Then the partial sums in the continuous coverage of the series, from a_1 to a_∞ can be reflected with the appropriate limits of integration: from a_1 to $a_{n>1}$, that is $\int_{x=0}^{x=n} f_n(x)dx$; from a_{n+1} to $a_{m>n} - \int_{x=n}^{x=m>n} f_n(x)dx$; from a_{m+1} to $a_\infty - \int_{x=m}^{\infty} f_n(x)dx$.

This implies the strict equality of the total sum of the series s to its initial s_n (“partial”, “final”), intermediate s_m (“middle”) and residual R_m parts

$$s = s_n + s_m + R_m. \tag{10}$$

If any of the parts is missing (there is no need to take it into account), then the remaining ones adjoin one another with the transition of the previous part upper limit to the next one lower limit, as established above. In this case, it is possible to determine one of the three sums by difference with the other two. The same possibility of difference calculation is applicable to the total sum (10).

Determining the equivalence relation of the series and the improper integral and establishing their isomorphism drastically simplifies computational procedures, since it allows one to find calculation formulas for all terms of equality (10)

$$s_n = \frac{1}{A}\int_0^n f_n(x)dx = \frac{1}{\frac{kT}{\triangle\varepsilon}(e^{\frac{\triangle\varepsilon}{kT}}-1)}\int_{x=0}^{x=n} e^{-\frac{(n-1)\triangle\varepsilon}{kT}}dx = \frac{1-e^{-\frac{n\triangle\varepsilon}{kT}}}{1-e^{-\frac{\triangle\varepsilon}{kT}}},$$

$$\Sigma P_n = \frac{s_n}{s} = \frac{1-e^{-\frac{n\triangle\varepsilon}{kT}}}{1-e^{-\frac{\triangle\varepsilon}{kT}}}\Bigg/\frac{1}{1-e^{-\frac{\triangle\varepsilon}{kT}}} = 1-e^{-\frac{n\triangle\varepsilon}{kT}},$$

$$s_m = \frac{1}{A}\int_{x=n}^{x=m>n} f_n(x)dx = -\frac{1}{A}\cdot\frac{kT}{\triangle\varepsilon}\Big|e^{-\frac{(x-1)\triangle\varepsilon}{kT}}\Big|_n^m = e^{-\frac{n\triangle\varepsilon}{kT}}\frac{1-e^{-\frac{(n-m)\triangle\varepsilon}{kT}}}{1-e^{-\frac{\triangle\varepsilon}{kT}}},$$

$$\Sigma P_m = \frac{s_m}{s} = e^{-\frac{n\triangle\varepsilon}{kT}}\frac{1-e^{\frac{(n-m)\triangle\varepsilon}{kT}}}{1-e^{-\frac{\triangle\varepsilon}{kT}}}\Bigg/\frac{1}{1-e^{-\frac{\triangle\varepsilon}{kT}}} = e^{-\frac{n\triangle\varepsilon}{kT}} - e^{-\frac{m\triangle\varepsilon}{kT}},$$

$$R_m = \frac{1}{A}\int_{x=m}^{\infty} f_n(x)dx = -\frac{1}{A}\cdot\frac{kT}{\triangle\varepsilon}\Big|e^{-\frac{(x-1)\triangle\varepsilon}{kT}}\Big|_m^\infty = \frac{e^{-\frac{m\triangle\varepsilon}{kT}}}{1-e^{-\frac{\triangle\varepsilon}{kT}}}, \tag{11}$$

$$\Sigma P_{R_m} = \frac{R_m}{s} = \frac{e^{-\frac{m\triangle\varepsilon}{kT}}}{1-e^{-\frac{\triangle\varepsilon}{kT}}}\Bigg/\frac{1}{1-e^{-\frac{\triangle\varepsilon}{kT}}} = e^{-\frac{m\triangle\varepsilon}{kT}}. \tag{12}$$

In this case, the ΣP_s total value is unity:

$$\Sigma P_s = \Sigma P_n + \Sigma P_m + \Sigma P_{R_m} = 1 - e^{\frac{-n\triangle\varepsilon}{kT}} + e^{\frac{-n\triangle\varepsilon}{kT}} - e^{\frac{-m\triangle\varepsilon}{kT}} + e^{\frac{-m\triangle\varepsilon}{kT}} = 1.$$

This indicates each relative sum probabilistic meaning, as follows from the Boltzmann distribution itself, which is a series of relative P_i values that sum to one. This result indicates the need for the constant joint presence of all series members as a whole.

The same is displayed by expressions for ΣP_n, ΣP_m and ΣP_{Rm}, containing $e^{\frac{-n\triangle\varepsilon}{kT}}$ and $e^{\frac{-m\triangle\varepsilon}{kT}}$ exponents. There are some arbitrary energy quantities $n\triangle\varepsilon$ and $m\triangle\varepsilon$ opposed to the kT system thermal energy state. And the corresponding probabilities of overcoming energy barriers $n\triangle\varepsilon$ or $m\triangle\varepsilon$ by the particles of the system (or not overcoming them at values $1-\Sigma P_n$ and $1-\Sigma P_m$).

This primarily refers to the activation energy, which expresses the probability of exceeding the barrier ε_a by the exponent $exp(-\varepsilon_a/(kT)$ in various chemical, physical, and mechanical processes [18]. The found energy quantity impact probability and its contribution to the process general conditions everything is not specified. In the rate constant, which was developed by Arrhenius in the 19^{th} century, the exponent included in it is treated as a thermodynamically determined quantity, without connection with the Boltzmann distribution, and even more so without analytical justification and expression.

2 Randomized particles concept

Much more modern is the randomized particles concept (RPC) proposed at the beginning of the 21^{st} century by the authors of [19, 20] which is entirely based on overcoming or not overcoming the natural thermal barriers of melting kT_m and boiling kT_b by its fractional (probabilistic) content of three energy particles classes: with energy less than kT_m – crystal-mobile (crm); with energy greater than kT_m, but less than kT_b – liquid-mobile (lqm); with energy more than kT_b – vapor-mobile (vm). The entire spectrum of these particles is present at any temperature and in any state of substance aggregation, in their probabilities sum it is unity with the difference from it to the fraction of crm-particles through P_{crm} – the fraction of kT_m superbarrier particles and from the difference with this fraction of vapor-mobile particles P_{vm} – the fraction liquid particles:

$$P_{crm} = 1 - exp(-kT_m) = 1 - exp(-T_m/T),$$

$$P_{lqm} = exp(-T_m/T) - exp(-T_b/T),$$

$$P_{vm} = exp(-T_b/T),$$

$$P_{crm} + P_{lqm} + P_{vm} = 1.$$

Each particle's energy variety plays its role in ensuring the corresponding state of aggregation stability and in preparing for the transition to it from other states, depending on the substance temperature, based on system-wide criteria for limiting stability, in particular, in proximity to the golden ratio.

In this case, the relationship between changes in the content of particles certain types and some substance physicochemical properties, for example, with the metal plasticity, the melts viscosity, and other properties, are revealed. With the advent of the randomized particles concept, finally, a general "zero model" of matter as a whole took place, and it goes back to the universal, and therefore fundamental, Boltzmann distribution according to the primary randomized (thermal) characteristic of matter — its kinetic energy. It is all the more important to strengthen the evidence-based part of RPC in order to eliminate some of its shortcomings.

First, from a physical point of view, the distribution is discrete both in content and form, since the energy is quantized. This quantum of energy should be present at least in a general form in the calculation formulas. Secondly, the possibility of expressing the partition function in a mathematically rigorous isomorphism terms of continuous and discrete distributions must necessarily be taken into account in the Boltzmann distribution, excluding the approximation in determining this sum. Thirdly, each energy class and energy spectrum as a whole must be expressed independently, directly, thereby proving the possibility of their isolation and unity in accordance with the superposition principle as a fundamental property of complex systems.

3 Isomorphism of discrete and continuous mappings of the Boltzmann distribution

The discreteness and continuity isomorphism analysis, which refers to accuracy expression of the partition function terms calculating, and along with this, the particles distribution over energy levels P_i with a further entropy definition, is necessary for a more rigorous Boltzmann distribution justification. In this case, the residual sum R_m (11) and its relative share P_{Rm} (12) play a special role. To determine the calculation accuracy of all discrete quantities, only the residual sum related to series all members a_n matters, so we use the index n' for the obtained absolute R_n and relative P_{Rn} expressions of the residual sum. Since it contains the terms closest to zero, which have a residual, almost negligible value, then it determines the calculating accuracy of the series sum δ (up to the residual sum ones)

$$\delta = \frac{R_n}{s} = P_{Rn} = e^{-\frac{n' \triangle\varepsilon}{kT}}. \qquad (13)$$

We obtain the calculation formula excluding from (13) the required number of the series terms n' to calculate their share with a given accuracy δ,

$$n' = -\frac{kT}{\triangle\varepsilon} ln\delta. \qquad (14)$$

The higher δ , the greater the number of terms of the series must be taken into account.

So, we limited ourselves to the results rounded to the nearest 10^{-4} when calculating the data in the Table. Substitute in (14) the used values $\triangle\varepsilon = 6.9032 \cdot 10^{-21} J \cdot \text{particle}^{-1}$, $T = 1000K$ and $k = 1.38064 \cdot 10^{-23} J \cdot \text{particle}^{-1} K^{-1}$, we obtain the value $n' = 18.4$. Rounding of the table data ends exactly in the interval $n = 1819$. Let's set a rougher accuracy limit $\delta = 0.001$, we get $n' = 13.8$, and this corresponds to the table data, where all values after $n = 13 \div 14$ cease to differ in the third decimal place. For control, we will take an even rougher accuracy $\delta = 0.01(1\%)$ and get $n' = 9.2$. We are convinced that in the interval $n = 9 \div 10$ the data difference ends by more than 1%, abs.

Table

Partition function members a_i, its accumulation $\Sigma_{i=1}^{i} a_i$, Boltzmann distribution P_i and its accumulation $\Sigma_{i=1}^{n} P_i$ at $T =$ 1000 K and $\triangle\varepsilon = \frac{1000k}{2}$, $J \cdot particle^{-1}$

i (n)	a_i	$\sum_{i=1}^{i} a_i$	P_i	$\sum_{i=1}^{i} P_i$
1	1	1	0.3933	0.3935
2	0.6065	1.6065	0.2386	0.6321
3	0.3679	1.9744	0.1448	0.7769
4	0.2231	2.1975	0.0878	0.8647
5	0.1353	2.3329	0.0532	0.9179
6	0.0821	2.4150	0.0323	0.9502
7	0.0498	2.4648	0.0196	0.9698
8	0.0302	2.4949	0.0119	0.9817
9	0.0183	2.5133	0.0072	0.9889
10	0.0111	2.5244	0.0044	0.9933
11	0.0067	2.5311	0.0026	0.9959
12	0.0041	2.5352	0.0016	0.9975
13	0.0025	2.5377	0.0010	0.9985
14	0.0016	2.5392	0.0006	0.9991
15	0.0009	2.5401	0.0004	0.9994
16	0.0006	2.5406	0.0002	0.9997
17	0.0003	2.5410	0.0001	0.9998
18	0.0002	2.5412	0.0001	0.9999
19	0.0001	2.5413	0.0000	0.9999
20	0.0001	2.5414	0.0000	1.0000

It is possible to estimate the requirement for the variation interval $\triangle\varepsilon$ by setting it to the smallest value $\triangle\varepsilon = 1.3806410^{-23} J \cdot \text{particle}^{-1}$. In this case, formula (14) takes the form

$$n' = -T \ln \delta. \tag{15}$$

We obtain the series terms required number $n' = 9210$, having set a practically acceptable calculation accuracy $\delta = 10^{-4}$, which would be difficult to implement without taking into account the discrete and continuous distributions isomorphism. Finally, using formula (15), one can determine the convergence condition, discrete and continuous distributions identification: since the latter of them are characterized by infinitely high accuracy, or vanishingly small error, this can be ensured by the condition $\delta \to 0$, under which the required number of series sum terms tends to infinity

$$\lim_{\delta\to 0} n' = \infty.$$

From formula (14) we release $\triangle\varepsilon$ and find its limit:

$$\triangle\varepsilon = -\tfrac{kT}{n'} \ln \delta, \quad \lim_{n'\to\infty} \triangle\varepsilon = 0.$$

Next, the isomorphism conditions (7) with respect to the equivalence relation A

$$\lim_{\triangle\varepsilon\to 0} A = \lim_{\triangle\varepsilon\to 0} \frac{kT}{\triangle\varepsilon}(e^{\frac{\triangle\varepsilon}{kT}} - 1) = \frac{0}{0}.$$

This uncertainty is revealed by L'Hopital's rule:

$$\lim_{\triangle\varepsilon\to 0} A = \lim_{\triangle\varepsilon\to 0} \frac{kT}{\triangle\varepsilon}(e^{\frac{\triangle\varepsilon}{kT}} - 1) = \lim_{\triangle\varepsilon\to 0} \frac{dkT(e^{\frac{\triangle\varepsilon}{kT}} - 1)d\varepsilon}{d\varepsilon} = \lim_{\triangle\varepsilon\to 0} \frac{kT}{kT} e^{\frac{\triangle\varepsilon}{kT}} = 1.$$

Thus, we can assume that establishing the discrete and continuous sequences isomorphism represents a broader scope of the problem than limiting the close proximity of both. And in any case, it involves both internal and external resources of the analyzed mathematical objects in solving the problem.

Conclusion

Establishing the series sum and an improper integral isomorphism requires knowledge or selection of a function that takes the series common term values at the points $x = n$. As such, a function is recommended that completely repeats the structure and the series common term form - a_n-model function, $f_n(x)$. The equivalence relation between the elements of the a_n-model function improper integral and the series of a common term is defined in an arbitrary unit interval and must satisfy the condition

$$A = \frac{\int_{x=n-1}^{n} f_n(x)dx}{a_n} \neq f(n).$$

In this case, it is possible to transfer A to each unit interval and to their entire set as a whole, ensuring complete mutual invertibility of both the two sets the elements and the series sum with an improper integral

$$\sum_{i=1}^{\infty} a_n \cong \frac{1}{A} \int_0^{\infty} f_n(x)dx.$$

The found isomorphism extends to finite sums of both convergent and divergent series.

Thanks to the established algorithm for identifying the series sum and an improper integral isomorphism, the Cauchy and Maclaurin series convergence integral criterion is developed in terms of proving not only convergence, but also determining the series sum.

The presented partition function is defined in its direct expression for the first time in many years of its discovery. Thanks to this, the concept of randomized particles received a more rigorous justification. This allowed the Boltzmann distribution itself to be expressed not in continuity approxima-tion, but taking into account its discreteness, that is, closer to its physical reality. At the same time, it became possible to single out its final and residual sums in the particle energy spectrum, and to associate the latter with a given accuracy of calculating the statistical sum, taking into account the necessary and this sufficient sum members number.

The decisive role of the a_n-model function is revealed in determining the isomorphism and accuracy of the calculation of compared infinite sequences as the most closely related to both the discrete and continuous sides of their isomorphism, automatically appearing along with the common term of the series and disappearing after the establishment or rejection of their isomorphism. Its modest role as a discreteness reducer and carrier to the improper integral of a continuous mapping is reminiscent of very fundamental isomorphic self-organization procedures in nature and in solving general scientific problems, consisting in maintaining their unity through the analytical connection of arbitrary elements of each of such sets.

The a_n-model function decisive role is to determine the isomorphism and compared infinite sequences calculation accuracy, closely related to both the discrete and continuous sides of their isomorphism, automatically appearing along with the series common term and disappearing after the establishment or rejection of their isomorphism. Its modest role as a discreteness reducer and carrier to the improper integral of a continuous mapping is reminiscent of the fundamental isomorphic self-organization procedures in nature and in solving general scientific problems, which consist in maintaining their unity through the analytical connection of such sets arbitrary each element.

Author Contributions

All authors contributed equally to this work.

Conflict of Interest

The authors declare no conflict of interest.

References

1 Федотов В.Х. О непрерывных и дискретных моделях эволюции / В.Х. Федотов, Н.И. Кольцов // Вестн. Казан. технолог. ун-та. — 2014. — № 17. — С. 9–13.

2 Парийская Е.Ю. Сравнительный анализ математических моделей и подходов к моделированию и анализу непрерывно-дискретных систем / Е.Ю. Парийская // Дифференциальные уравнения и процессы управления. — 1997. — № 1. — С. 91–120.

3 Kvasnikov V.P. Technology for restoring functional dependencies to determine reliability parameters / V.P. Kvasnikov, S.V. Yehorov, T.Yu. Shkvarnytska // Bulletin of the Karaganda University. Mathematics series. — 2021. — № 1(101). — С. 78–86. https://doi.org/10.31489/2021m1/78-86

4 Битюков В.И. Изоморфизм. Математический энциклопедический словарь / В.И. Битюков, А.Н. Колмогоров. — М.: Сов. энцикл., 1988. — 224 с.

5 Бронштейн И.Н. Справочник по математике для инженеров и учащихся втузов / И.Н. Бронштейн, К.А. Семендяев. — М.: Наука, 1986. — 544 с.

6 Малышев В.П. О взаимосвязи и соразмерности дискретных и непрерывных зависимостей / В.П. Малышев, А.М. Макашева, Ю.С. Зубрина (Красикова) // Докл. НАН РК. — 2016. — № 1. — С. 49–56.

7 Малышев В.П. Распределение Больцмана как бесконечная последовательность и сходящийся ряд / В.П. Малышев, Ю.С. Зубрина, А.М. Макашева // Вестн. НАН РК. — 2017. — № 1. — С. 49–58.

8 Malyshev V.P. Quantization of particle energy in the analysis of the Boltzmann distribution and entropy / V.P. Malyshev, Yu.S. Zubrina, A.M. Makasheva // Journal of Mathematics and System Science. — 2017. — Vol. 7. — P. 278–288. https://doi.org/10.17265/2159-5291/2017.10.002

9 Malyshev V.P. Analytical determination of the statistic Sum and the Boltzmann distribution / V.P. Malyshev, Yu.S. Zubrina, A.M. Makasheva // Abstracts of the XXI International Conference on Chemical Thermodynamics in Russia. — Novosibirsk: Akademgorodok, 2017. — P. 74.

10 Малышев В.П. Распределение и энтропия Больцмана как бесконечные сходящиеся последовательности / В.П. Малышев, А.М. Макашева, Ю.С. Красикова // Вестн. Караганд. ун-та. Сер. Физика. — 2018. — № 3(91). — С. 42–58.

11 Фихтенгольц Г.М. Курс дифференциального и интегрального исчисления / Г.М. Фихтенгольц. — Т. 2. — М.: Физматлит, 2003.

12 Graham R.L. Concrete Mathematics / R.L. Graham, D.E. Knuth, O. Patashnik. — Massachusetts: Addison-Wesley, 2nd ed., 1994. — 604 p.

13 Бермант А.Ф. Краткий курс математического анализа / А.Ф. Бермант. — М.: Наука, 1964. — С. 576–578.

14 Ramnath S. On the isomorphism of expressions / S. Ramnath, P.Y. Zhao // Information Processing Letters. — 2000. — Vol. 74. — No. 3-4. — P. 97–102.

15 Keshvardoost K. Definable Isomorphism Problem / K. Keshvardoost, B. Klin, S. Lasota, J. Ochremiak, S. Torunczyk // Logical methods in Computer Science. — 2019. — Vol. 15. — No. 4. — P. 14–19.

16 Ibraev Sh.Sh. Cohomology of simple modules for algebraic groups / Sh.Sh. Ibraev, L.S. Kainbaeva, S.K. Menlikhozhayeva // Bulletin of the Karaganda University. Mathematics series. — 2020. — № 1(97). — C. 37–43. https://doi.org/10.31489/2020M1/37-43

17 Dummit D.S. Abstract algebra / D.S. Dummit, R.M. Foote. — Wiley: Hoboken, NJ, 2004. — 946 p.

18 Малышев В.П. Распределение Больцмана как основа универсального выражения энергии активации вязкого течения, химических реакций и механического разрушения / В.П. Малышев, А.М. Макашева // Цветные металлы. — 2018. — № 10. — С. 6–12. https://doi.org/10.17580/tsm.2018.10.01

19 Малышев В.П. Концепция хаотизированных частиц как основа единого отображения твердого, жидкого и газообразного состояний вещества / В.П. Малышев, А.М. Нурмагамбетова (Макашева) // Вестн. Казах. нац. ун-та. Сер. Химия. — 2004. — № 3. — С. 53–67.

20 Malyshev V.P. Invariants of ratio of crystal-mobile, liquid-mobile, and vaporized chaotized particles in solid, liquid, and gas states of substance / V.P. Malyshev, A.M. Makasheva, L.A. Bekbaeva // Bulletin of the University of Karaganda – Chemistry — 2021. — No. 4(104). — P. 69–78. https://doi.org/10.31489/2021Ch4/69-78

Қатардың қосындысы мен меншіксіз интегралдың изоморфизмі туралы теоремалар

В.П. Малышев[1], С.Ш. Кажикенова[2], А.М. Мақашева[1], А.Ш. Кажикенова[3]

[1] *Ж. Әбішев атындағы Химия-металлургия институты, Қарағанды, Қазақстан;*
[2] *Ә. Сағынов атындағы Қарағанды техникалық университеті, Қарағанды, Қазақстан;*
[3] *Академик Е.А. Бөкетов атындағы Қарағанды университеті, Қарағанды, Қазақстан*

Мақалада дискретті және үздіксіз тәуелділіктердің байланысы туралы мәселе зерттелген. Коши қатарының үйлесімділігінің кеңейтілген интегралдық белгісі негізінде a_n қатарының жалпы мүшесінің эквиваленттік қатынасы және олардың өзгеруінің бірлік интервалы аралығындағы a_n-тәрізді функцияның орташа интегралдық шамасы арқылы қатардың соңғы және толық қосындыларын анықтау алгоритмі жасалды. Больцман үлестіріміндегі статистикалық қосынды үшін мұндай сомаларды анықтау мысалдары келтірілген, олар алғаш рет a_n-тәрізді функция арқылы тікелей көрсетілді. Бұл осы соманың белгілі бір дәлдігімен берілген мәнге дейін қатардың қосындысын жинақтау үшін есептеулер жүргізу қажеттілігін жояды. Сонымен қатар, бұл жағдайда энергияның өзгеру аралығын кез келген дәлдікпен өзгертуге мүмкіндік береді. Жүргізілген зерттеулер технологиялық процестердегі жылу энергиясының жоғалуын анықтайтын энтропияны есептеу үшін Больцманның таралуын (энергия спектрін) тікелей қолдана отырып, физика мен материалтану саласындағы теориялық және практикалық мәселелерді шешуге мүмкіндік береді.

Кілт сөздер: изоморфизм, қатар қосындысы, меншіксіз интеграл, бірлік интервал, эквиваленттік қатынас.

Теоремы об изоморфизме суммы ряда и несобственного интеграла

В.П. Малышев[1], С.Ш. Кажикенова[2], А.М. Макашева[1], А.Ш. Кажикенова[3]

[1] *Химико-металлургический институт имени Ж. Абишева, Караганда, Казахстан;*
[2] *Карагандинский технический университет имени Абылкаса Сагинова, Караганда, Казахстан;*
[3] *Карагандинский университет имени академика Е.А. Букетова, Караганда, Казахстан*

Исследован вопрос о взаимосвязи дискретных и непрерывных зависимостей. На основе расширенного интегрального признака сходимости ряда Коши разработан алгоритм определения конечной и полной сумм ряда через отношение эквивалентности общего члена ряда a_n и среднеинтегральной величины a_n-образной функции в пределах единичного интервала их изменения. Приведены примеры определения таких сумм для статистической суммы в распределении Больцмана, впервые непосредственно выраженной через a_n-образную функцию. Это исключает необходимость проведения расчетов по накоплению суммы ряда до значения, которое задается определенной точностью этой суммы. Кроме того, она позволяет в данном случае варьировать интервал вариации энергии с любой заданной точностью. Проведенные исследования позволяют решать как теоретические, так и практические задачи физики и материаловедения, непосредственно используя распределение (энергетический спектр) Больцмана для расчета энтропии, определяющей потери тепловой энергии в технологических процессах.

Ключевые слова: изоморфизм, сумма ряда, несобственный интеграл, единичный интервал, отношение эквивалентности.

References

1 Fedotov, V.Kh., & Koltsov, N.I. (2014). O nepreryvnykh i diskretnykh modeliakh evoliutsii [On continuous and discrete models of evolution]. *Vestnik Kazanskogo tekhnologicheskogo universiteta — Bulletin of the Kazan Technological University,* 17, 9–13 [in Russian].

2 Pariiskaia, E.Yu. (1997). Sravnitelnyi analiz matematicheskikh modelei i podkhodov k modelirovaniiu i analizu nepreryvno-diskretnykh sistem [Comparative analysis of mathematical models and approaches to modeling and analysis of continuous-discrete systems]. *Differentsialnye uravneniia i protsessy upravleniia — Differential Equations and Control Processes,* 1, 91–120 [in Russian].

3 Kvasnikov, V.P., Yehorov, S.V. & Shkvarnytska, T.Yu. (2021). Technology for restoring functional dependencies to determine reliability parameters. *Bulletin of the Karaganda University. Mathematics series,* 1(101), 78–86. https://doi.org/10.31489/2021M1/78-86

4 Bitiukov, V.I., & Kolmogorov, A.N. (1988). *Izomorfizm. Matematicheskii entsiklopedicheskii slovar [Isomorphism. Mathematical Encyclopedic Dictionary].* Moscow: Sovetskaia entsiklopediia [in Russian].

5 Bronshtein, I.N., & Semendiaev, K.A. (1986). S*pravochnik po matematike dlia inzhenerov i uchashchikhsia vtuzov [Handbook of mathematics for engineers and students of technical universities].* Moscow: Nauka [in Russian].

6 Malyshev, V.P., Makasheva, A.M., & Zubrina, Yu.S. (2016). O vzaimosviazi i sorazmernosti diskretnykh i nepreryvnykh zavisimostei [On the relationship and proportionality of discrete and continuous dependencies]. *Doklady Natsionalnoi akademii nauk Respubliki Kazakhstan — Reports of the National Academy of Sciences of the Republic of Kazakhstan,* 1, 49–56 [in Russian].

7 Malyshev, V.P., Zubrina, Yu.S., & Makasheva, A.M. (2017). Raspredelenie Boltsmana kak beskonechnaia posledovatelnost i skhodiashchiisia riad [The Boltzmann distribution as an infinite sequence and a convergent series]. *Vestnik Natsionalnoi akademii nauk Respubliki Kazakhstan — Bulletin of the National Academy of Sciences of the Republic of Kazakhstan,* 1, 49–58 [in Russian].

8 Malyshev, V.P., Zubrina, Yu.S., & Makasheva, A.M. (2017). Quantization of particle energy in the analysis of the Boltzmann distribution and entropy. *Journal of Mathematics and System Science, 7,* 278–288. https://doi.org/10.17265/2159-5291/2017.10.002

9 Malyshev, V.P., Zubrina, Yu.S., & Makasheva, A.M. (2017). Analytical determination of the statistic Sum and the Boltzmann distribution. *Abstracts of the XXI International Conference on Chemical Thermodynamics in Russia,* 74.

10 Malyshev, V.P., Makasheva, A.M., & Krasikova, Yu.S. (2018). Raspredelenie i entropiia Boltsmana kak beskonechnye skhodiashchiesia posledovatelnosti [Distribution and entropy of Boltzmann as infinite convergent sequences]. *Vestnik Karagandinskogo universiteta. Seriia Fizika — Bulletin of Karaganda University, Physics series,* 3(91), 42–58 [in Russian].

11 Fikhtengolts, G.M. (2003). *Kurs differentsialnogo i integralnogo ischisleniia [Course of differential and integral calculus].* Moscow: Fizmatlit [in Russian].

12 Graham, R.L., Knuth, D.E., & Patashnik, O. (1994). *Concrete Mathematics,* 2nd ed. Massachusetts: Addison-Wesley.

13 Bermant, A.F. (1964). *Kratkii kurs matematicheskogo analiza [A Short Course in mathematical analysis].* Moscow: Nauka [in Russian].

14 Ramnath, S., & Zhao, P.Y. (2000). On the isomorphism of expressions. *Information Processing Letters, 74* (3–4), 97–102.

15 Keshvardoost, K., Klin, B., Lasota, S., Ochremiak, J., & et al. (2019). Definable Isomorphism Problem. *Logical methods in Computer Science, 15* (4), 14.

16 Ibraev, Sh.Sh., Kainbaeva, L.S., & Menlikhozhayeva, S.K. (2020). Cohomology of simple modules for algebraic groups. *Bulletin of the Karaganda University. Mathematics series, 1* (97), 37–43. https://doi.org/10.31489/2020M1/37-43

17 Dummit, D.S., & Foote, R.M. (2004). *Abstract algebra.* Hoboken: NJ, Wiley.

18 Malyshev, V.P., & Makasheva, A.M. (2018). Raspredelenie Boltsmana kak osnova universalnogo vyrazheniia energii aktivatsii viazkogo techeniia, khimicheskikh reaktsii i mekhanicheskogo razrusheniia [Boltzmann distribution as the basis for a universal expression of the activation energy of viscous flow, chemical reactions and mechanical destruction]. *Tsvetnye metally — Non-ferrous metals,* 10, 6–12 [in Russian]. https://doi.org/10.17580/tsm.2018.10.01

19 Malyshev, V.P., & Makasheva, A.M. (2004). Kontseptsiia khaotizirovannykh chastits kak osnova edinogo otobrazheniia tverdogo, zhidkogo i gazoobraznogo sostoianii veshchestva [The concept of randomized particles as the basis for a unified display of solid, liquid and gaseous states of matter]. *Vestnik Kazakhskogo natsionalnogo universiteta. Seriia Khimiia — Bulletin of the Kazakh National University, Chemistry series, 3*(35), 53–67 [in Russian].

20 Malyshev, V.P., Makasheva, A.M., & Bekbaeva, L.A. (2021). Invariants of ratio of crystal-mobile, liquid-mobile, and vaporized chaotized particles in solid, liquid, and gas states of substance. *Bulletin of the University of Karaganda – Chemistry,* 4(104), 69–78. https://doi.org/10.31489/2021Ch4/69-78

*Author Information**

Vitalyi Pavlovich Malyshev — Doctor of technical sciences, Professor, Chief Researcher at the Laboratory of Entropy and Information Analysis of Complex Physicochemical Systems, Abishev Chemical and Metallurgical Institute, 63 Ermekov street, Karaganda, 100009, Kazakhstan; e-mail: *eia_hmi@mail.ru*; https://orcid.org/0000-0002-3996-1533

Saule Sharapatovna Kazhikenova — Doctor of technical sciences, Professor, Head of the Department of Higher Mathematics, Abylkas Saginov Karaganda Technical University, 56 Nursultan Nazarbayev Avenue, Karaganda, 100000, Kazakhstan; e-mail: *sauleshka555@mail.ru*; https://orcid.org/0000-0002-6937-1577

Astra Mundukovna Makasheva (*corresponding author*) — Doctor of technical sciences, Professor, Head of the Laboratory of Chief Researcher at the Laboratory of Entropy and Information Analysis of Complex Physicochemical Systems, Abishev Chemical and Metallurgical Institute, 63 Ermekov street, Karaganda, 100009, Kazakhstan; e-mail: *astra_mun@mail.ru*; https://orcid.org/0000-0003-2249-3435

Aigul Sharapatovna Kazhikenova — Candidate of technical sciences, Associate Professor of the Department of Higher Mathematics, Karaganda Buketov University, 28 Universitetskaya street, Karaganda, 100028, Kazakhstan; e-mail: *aigul-kazhikenova@mail.ru*; https://orcid.org/0000-0003-4053-1546

*The author's name is presented in the order: First, Middle and Last Names.