ФИЗИКА

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AXIOMATIC PRINCIPLES AND DETAILED BALANCE

Abstract. This article presents an analysis of scientific papers and research on axiomatic principles and detailed balance, we are convinced that even today, in accordance with modern requirements, there is still a need to address axiomatic principles and detailed balance, methods and methods for their study.

As mentioned earlier, the axiomatics of statistical physics is reduced to the principle of equal probability of the existence of an equilibrium closed physical system in all microstates accessible to it. This postulate, in turn, suggests that the time-averaged probability of the direct and reverse transition of the system between two selected groups of microstates in the accessible region of the phase space must be the same in both directions (this follows from the definition of an equilibrium state, which contains the requirement of stationarity).

In fairness, it should be noted that the principle of detailed balance is not a consequence of the axiomatic principles of statistical physics, and therefore, strictly speaking, is not required to be applied within the framework of this axiomatics. There are situations and outcomes we have given in this article, when the principle of equal probability of available microstates in a closed system is satisfied, but the principle of detailed statistical equilibrium is not.

Key words: axiomatics, closed system, postulate, equilibrium, microstates.

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Аксиоматикалық принциптер және егжей-тегжейлі тепе-теңдік күйі

Аңдатпа. Бұл мақалада аксиоматикалық принциптер мен егжей-тегжейлі тепе-теңдік туралы ғылыми еңбектер мен зерттеулердің талдауы берілген, біз бүгінгі күннің өзінде заманауи талаптарға сәйкес аксиоматикалық принциптер мен егжей-тегжейлі тепе-теңдік, оларды зерттеу әдістері мен әдістерін шешу қажеттілігінің әлі де бар екеніне сенімдіміз.

Бұрын айтылғандай, статистикалық физика аксиоматикасы оған қол жетімді барлық микрокүйлерде тепе-теңдік тұйық физикалық жүйенің болуының тең ықтималдылығы принципіне келтірілген. Бұл постулат, өз кезегінде, фазалық кеңістіктің қол жетімді аймағында микрокүйлердің екі таңдалған топтары арасындағы жүйенің тікелей және кері ауысуының уақыт бойынша орташа ықтималдығы екі бағытта бірдей болуы керек деп болжайды (бұл анықтамадан туындайтын тұжырым стационарлық талапты қамтитын тепе-теңдік күй болып табылады).

Әділдік үшін айта кету керек, егжей-тегжейлі тепе-теңдік принципі статистикалық физиканың аксиоматикалық принциптерінің салдары емес, сондықтан, қатаң айтқанда, бұл аксиоматика шеңберінде қолдану талап етілмейді. Жабық жүйедегі қол жетімді микрокүйлердің тең ықтималдылығы принципі орындалғанымен, егжей-тегжейлі статистикалық тепе-теңдік принципі орындалмаған жағдайда, біз осы мақалада келтірген жағдайлар мен нәтижелер бар.

Кілт сөздер: аксиоматика, тұйық жүйе, постулат, тепе-теңдік, микрокүйлер.

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Анализ выполнимости аксиоматических принципов статистической физики

Аннотация. В данной статье представлены анализ научных работ и исследования аксиоматические принципы и детальное равновесие, мы убедились, что и сегодня, в соответствии с современными требованиями, по-прежнему существует необходимость решения аксиоматические принципов и детальное равновесие, методов и способов их исследование.

Как уже говорилось ранее, аксиоматика статистической физики сводится к принципу равно вероятности пребывания равновесной замкнутой физической системы во всех доступных ей микросостояниях. Данный постулат, в свою очередь, предполагает, что средняя по времени вероятность прямого и обратного перехода системы между двумя выделенными группами микросостояний в доступной области фазового пространства – должна быть одинакова в обоих направлениях (это следует из определения равновесного состояния, которое содержит требование стационарности).

Справедливости ради следует заметить, что принцип детального равновесия не является следствием аксиоматических принципов статистической физики, и потому, строго говоря, не обязателен к применению в рамках указанной аксиоматики. Возможны ситуации и исходы мы привели в данной статье, когда принцип равно вероятности доступных микросостояний в замкнутой системе выполняется, а принцип детального статистического равновесия – нет.

Ключевые слова: аксиоматика, замкнутая система, постулат, равновесие, микросостояния.

Introduction

As you know, one of the main goals of any real natural science (for example, any branch of physics) is to generalize the previously accumulated empirical (experimental) experience. Such generalizations, usually expressed in the form of mathematical dependencies, allow predicting the behavior of certain objects that are the subject of the corresponding science. Thus, these mathematical dependencies are nothing more than empirical regression equations that more or less successfully approximate the actual characteristics of the studied natural phenomena. However, only the results of regression analysis of experimental data are not enough to create very complex mathematical models that go beyond primitive empiricism. Often, describing the studied objects in depth and in detail, it will be necessary to involve some additional fundamental concepts (main principles). It is impossible to prove the correctness of using these concepts within the scientific discipline based on them. Therefore, the corresponding principles have the character of certain presuppositions a priori assumed to be self-evident. These postulates form the axiomatics of the science based on them [1]. From the above, the reliability of the results of modeling certain real phenomena is determined both by the quality of the approximation within the framework of creating the corresponding «empirical regression equations» and by the validity of using the dependencies found to study something. subject area. The quality of the approximation depends on the amount of previously collected empirical material and the capabilities of the regression analysis method involved in its processing. The validity of using the obtained mathematical dependencies is characterized by the correctness of using the axiomatics of the scientific apparatus to model a clearly defined natural phenomenon. The validity of axiomatics is explained by the fact that the amount of available experimental data does not yet determine the limits of applicability of the mathematical models based on them: it does not matter how reliable this or that regression approximation is found. for some previously studied subject area, if there is a phenomenon currently under consideration, it certainly does not belong to this field. Thus, the existing experience of creating scientific theories says: an arbitrarily large amount of empirical information does not guarantee the transition to the methodological quality of conclusions based on them. One of the most obvious examples of the limited applicability of the main postulates of some scientific disciplines is the glorious (over two centuries) history of the development of classical mechanics based on Newton's very reasonable and intuitive assumptions about properties. Space and time. However, like any physical theory, Newtonian physics proved adequate to reality only within the framework of the applicability of its basic hypotheses. The subsequent emergence of relativistic physics (Michelson's experiment) and quantum mechanics (the «ultraviolet crash») was another proof of this situation: no theory can claim the role of absolute truth, even if it fits perfectly with most of the known empirical data.

Another example of this type is the hypothesis of the fundamental indivisibility of atoms, based on the vast experience of mankind in the relevant field. This experience summed up empirical knowledge accumulated over three thousand years. Many centuries-long attempts of alchemists to carry out the so-called «transmutation» (the transformation of some chemical elements into others) have completely failed, because these actions are carried out with the help of chemical reactions, i.e. application of atomistic theory. Moreover, the obvious futility of long-term efforts discredited even the idea of the reality of achieving this goal. Only the discovery of the so-called nuclear reactions made it possible to realize what was considered impossible for several decades.

Everything mentioned above in this article is very trivial and known. However, experience shows that people tend to make their experiences absolute.

Due to the subjective nature of the perception of scientific knowledge, it is preferable to emphasize the following important situation here: the conclusions of any scientific discipline, even if they are pathetically declared as «basic laws of nature», don't just hang in the air like a Cheshire Cat grin. These conclusions are always based on fully known axiomatics and a fairly limited (but possibly very large) amount of empirical information. These conditions fundamentally limit the limits of application of the results of certain scientific analysis. The very fact of such limitations is an integral feature of the scientific method of cognition [2].

In this article, an attempt is made to specify the limits of application of those axiomatic principles that form the formalism of statistical physics. The obtained conclusions, of course, also refer to the limits of the correct application of thermodynamics.

The question of the validity of the application of this axiomatic in certain specific cases is a matter of fundamental importance and has been the subject of the closest consideration and many discussions since the emergence of statistical physics (mid-19th century). The interest in the above issue is due to the following two reasons:

1. The axiomatics of statistical physics are indeed not free from serious contradictions, which in many cases are of a qualitative nature. Most of these contradictions are related to attempts to justify the irreversibility of real physical processes, a posteriori proof of Boltzmann's H-theorem (a

statistical analogue of the second law of thermodynamics), etc., he writes in his book «Statistical Mechanics» [p. 3]: «Fundamentals of statistical mechanics». Physics takes a leading place among real sciences, and statistical mechanics is one of its main branches. It may surprise the reader if we say that there are many ambiguities in the justification of statistical mechanics. Working in this field, the author of this book feels a little uncomfortable, but it really is.

2. It is clear that such macroscopic phenomena are indisputable in nature, their very existence clearly contradicts, for example, the above-mentioned Boltzmann's H-theorem. Of course, we are talking about the nature of dynamic processes observed by astronomers on a galactic and metagalactic scale. In almost every physics textbook you can find a chapter devoted to testing the theory of the heat death of the universe. This criticism itself ranges from a declarative statement about the openness of the Universe as a physical system (Boltzmann's H-theorem does not apply to such objects), to complex attempts to somehow explain the actually observed phenomena within the framework of the laws of statistical physics. thermodynamics: it has come a long way – from Boltzmann's simple fluctuation hypothesis (more than a century ago) to the most complex modern models of the Universe. Below is a typical quote from the textbook «Thermodynamics and Statistical Physics» [4]. The worldwide historical result of the work of thermodynamicists in the second half of the 19th century was the discovery of the second law of thermodynamics, the conditions for the equilibrium and stability of an isolated thermodynamic system.

The most important results in the creation and formulation of the second law of thermodynamics belong to Clausius. In 1865, he spread the second law of thermodynamics, the law of increase of entropy, to the universe and said, «The energy of the world is constant. The entropy of the universe tends to the maximum».

By unreasonably extending the second law of thermodynamics and applying it to the universe, Clausius made the wrong philosophical conclusions. This was the basis for the theory of the heat death of the universe. Clausius and Thomson argued that when thermal equilibrium is reached in the Universe, thermal death occurs, all spontaneous processes cease, and the Universe freezes in lifeless stillness.

Boltzmann struggled with the theory of the heat death of the Universe based on probabilistic and statistical views. It was objected that, although the Universe is close to equilibrium, its individual parts have enormous deviations, the dimensions of which are large compared to the dimensions of the surrounding man and the world. he observes and is long incomparable to the length of his life. But at the same time, these fluctuating formations are infinitesimally small compared to the infinitely large and eternally existing Universe.

However, these conclusions cannot be recognized as correct, because from the point of view of the world around us, the idea of the probability of such large deviations in the Universe is equivalent to the idea of improbability.

According to the Boltzmann hypothesis, new star formation observed in the visible part of the Universe is very unlikely. Currently, various views are being put forward to clarify the existing contradiction.

However, without going into detail about the disagreements on this point, we limit ourselves to the following remarks. First, the currently available experimental data show that the theory of the heat death of the Universe is incorrect; all human experience confirms that there is a continuous development in the world around us, and there are no grounds or even hints to believe that the processes are slowing down in the direction of stopping. Science shows the continuous circulation and movement of matter, the development and change of forms of movement, the continuous transformation of some types of matter into others, and their infinite diversity. The meritorious work of astronomers and astrophysicists is the proof that in the Universe there are continuous complex and diverse connections between stars and interstellar matter, which lead to the continuous formation, development and destruction of star structures, galaxies, and worlds [5].

Thus, regarding Boltzmann's H-theorem, for example, it is impossible to make an analogy with Fermat's theorem: they say that a rigorous proof has not yet been found, however, there are no exceptions to the rules under consideration. Such a situation gives reason to believe that the emergence of these evidences is only a matter of time1. On the contrary, the data of astrophysical observations show that the cases where the discussed conclusions of statistical physics are fulfilled on the scale of the Universe should be considered as exceptions.

Here, unfortunately, it is not possible to give a detailed overview of the works on the interesting topic. Therefore, we will limit ourselves to stating the obvious fact that we live in a world that is much more complex than we imagine based on current model concepts of statistical physics and thermodynamics. The author made a theoretically based assumption that there are some types of physical systems that cannot be adequately described within the limits of application of the axiomatics of the above-mentioned scientific disciplines, even on a scale that is not large than universal. The present work [6] is dedicated to the initial phase of the study of these systems, carried out within the framework of the Euler research project.

Research methods

The axiomatics of the theory of non-equilibrium processes includes a number of different postulates, the most famous of which is called the molecular chaos hypothesis (Stoßzahlansatz). This hypothesis was put forward by L. Boltzmann as an objection to I. Loschmidt (paradox of reversibility – Umkereinward, 1876) and E. Zermelo (paradox of recurrence based on the Poincaré recurrence theorem – Wiederkereinvand, 1896). The H-theorem introduced by Boltzmann into the apparatus of statistical physics as a functional analogue of the second law of thermodynamics [7].

A detailed analysis of the axiomatics of the theory of non-equilibrium processes is not the subject of this work. However, it should be noted that the molecular chaos hypothesis, like Boltzmann's ergodic hypothesis, contradicts set theory in other matters. In classical molecular-kinetic theory (as opposed to quantum theory), the dynamics of particles is strictly defined. The strict Laplace formalism of describing a physical system completely excludes the possibility of any «backlash» in the parameters of particle motion, which can manifest itself (and accumulate) as a result of, for example, the collision of these particles with each other. These conclusions do not depend on the number of particles in the system and the time of its observation. Any interminism in the relaxation of particle momentum and (or) energy as a result of individual scattering events is by definition absent, i.e., it is a zero-dimensional set. The sum of any number of zeros is always zero because «you can't get something out of nothing». Thus, the state of a classical system is always strictly defined [8].

In asymptotic combinatorics, there are various methods for studying problems related to the behavior of Young's tables for different Markov processes. These methods include, in particular, the use of the Robinson-Schoenstedt-Knuth (RSK) algorithm and the Schutzenberger transformation [9].

The sequence generators of the following Markov processes were implemented in this work:

- Richardson process in 2D and 3D Young and Schur graphs;
- Plancherel process in two-dimensional Young and Schur graphs;
- is a pseudo-Plancherel process on a three-dimensional Young's graph.

Since the dimensions of Young's diagrams grow exponentially, it is necessary to normalize them in a certain way in order to study their asymptotic properties. A normalization method for two-dimensional standard Young's diagrams is introduced in [10]. Formulas for normalized measurements on the Schur graph [11] and the three-dimensional Yang graph [12] were proposed within the framework of this dissertation [13].

There are various methods for modeling random sequences of Young's diagrams with Plancherel distribution. In particular, [14], such circuits were created using the Robinson-Schensted-Knuth algorithm. In this dissertation research, this problem was solved by introducing a Markov chain in the Yang graph, which allowed the creation of a sequence of Yang diagrams of a much larger length.

A method based on the use of the Schutzenberger transformation was used to calculate the cotranslational probabilities of the central stochastic process in the three-dimensional Young's graph. In the dissertation, its randomized modification was proposed, the use of which made it possible to create random Young tables of the given form with a uniform random distribution [15].

Results and discussion

The study of the asymptotic behavior of the normalized dimensions of Young's diagrams with maximum dimensions is an interesting problem in asymptotic representation theory. This asymptotics describes the growth of the weights of maximal irreducible representations of a symmetric group.

[11] introduced the concept of the normalized size of standard Young's diagrams and obtained two-way estimates for the normalized dimensions of Plancherel dimension characteristic diagrams and for maximum dimension diagrams. In addition, the same paper proposed a conjecture (yet not fully proven) about the convergence of normalized dimensions for both normal Plancherel diagrams and diagrams with maximal dimensions. Verification of the implementation of these hypotheses with the help of computer experiments [12]. The results of the experiments described in these articles give reason to believe that the Vershik-Kerov hypothesis is correct. Approximate estimates of normalized size limits are also given in [13].

In the article [14], the model of the multipart process, known in modern literature as TASEP (Total Asymmetric Simple Exclusion Process), was studied. TASEP is modeled by growing Younggas diagrams according to Richardson statistics (see 1.7.2). The probability distribution density corresponding to this process was studied, and a formula for the limiting form of Richardson-distributed Young's diagrams was derived. In this work, we study the asymptotic growth of normalized dimensions with the help of computer experiments.

Since the actual dimensions of Young's diagrams grow exponentially with their size, it is convenient to use their normalization to study the asymptotic order of dimensions of Young's diagrams. The normalized size csta of the standard λ diagram presented in [11] is determined by the following formula:

$$c_{sta}(\lambda)=\frac{-2}{\sqrt{n}}\ln\frac{\dim\lambda}{\sqrt{n!}}, \tag{1}$$

where n is the size of the chart, dimλ is the size of the chart.

It was proved [11] that the values of the normalized dimension are limited to the range [c0,c1]:

$$c_0=\frac{2}{\pi}-\frac{4}{\pi^2}\approx 0.2313, c_1=\frac{2\pi}{\sqrt{6}}\approx 2.5651. \tag{2}$$

It was also suggested that the normalized sizes of charts with maximum dimensions approach a certain limit. This assumption has not been proven, but many computer experiments give some confidence in its truth [15]. For the size of the rigid diagram [16], the following normalization was used:

$$c_{str}(\lambda)=-\frac{\ln\dim(\lambda)-\ln\sqrt{n!}+\frac{\ln 2}{2}\cdot n}{\sqrt{n}}. \tag{3}$$

In quantum physics, it is also believed that there is an equality of probabilities 2 in time of direct and reverse transitions between two distinguished microstates. This equality is realized within the framework of the so-called Pauli-Luders CPT theorem: if in nature there is a probability of a certain process occurring, then with exactly the same probability amplitude, a certain conjugated process can also be realized in it, in which the particles are replaced by the corresponding antiparticles, the projections of their spins and pulses changed sign, and the initial and final positions of the particles in the geometric space were reversed. In the present paper, it is appropriate to use the concept of T-invariance, which is less rigorous than the CPT theorem, meaning the symmetry of the probability of a physical process occurring with respect to the inversion of the sign of time.

If electron scattering occurs elastically, i.e., without energy $\left(\varepsilon = m\cdot v^2/2 = \varepsilon' = m\cdot v'^2/2\right)$, то $v = v'$. . In this case, when equilibrium

$$\left(\frac{\partial f}{\partial t}\right)_{\text{ст}} = 0 = f_0(v)\cdot[1-f_0(v)]\cdot\int\left\{W(\mathbf{v}',\mathbf{v})-W(\mathbf{v},\mathbf{v}')\right\}\cdot d\mathbf{v}'. \qquad 4$$

Hence it follows that $W(\mathbf{v}',\mathbf{v}) = W(\mathbf{v},\mathbf{v}')$,

i.e., the probabilities of direct and reverse transitions are the same. Condition (4) is called the principle of detailed balance. It is obvious that relation (4), referring to the elementary act of scattering, does not depend on whether the electron gas is in an equilibrium or non-equilibrium state. In the book «Fundamentals of Quantum Mechanics» by D.I. Blokhintsev, the above – described equal probability of direct and reverse transitions between different states of a quantum physical system is referred to as the principle of detailed balance. This principle is defined here on the basis of consideration of the act of particle scattering in the framework of model representations of Heisenberg's matrix mechanics:

$$\hat{S} = \hat{S}(+\infty,-\infty) = \lim_{\substack{t\to+\infty \\ t_0\to-\infty}} \hat{S}(t,t_0) \qquad 5$$

where $\hat{S}$ is a unitary operator representing the so–called scattering matrix. The matrix elements of the operator $\hat{S}$ (t,t_0) determine the probabilities of transitions from one quantum state to another: $P_{nm}(t,t_0)=|Snm(t,t0)|^2$ $Pnm(t,t0)$– state L = Ln (time 0t) to state L = Lm (time t). It is this approach that is most adequate for the case when a free particle performs an induced (as a result of an act of scattering on an obstacle) transition from one remote (t0 → –∞) pure1 state to another remote (t → +∞) pure state, which, for example, characteristic of the case of Fraunhofer diffraction.

Conclusion

If any closed system is in its most probable macroscopic state, then an axiomatic principle of statistical physics postulates an equal probability of finding this system in any of the microstates available to it. This, in turn, means the existence of a dynamic equilibrium between each pair of regions defined in the phase space of the specified system: the time-averaged probability of the system transition from one region to another must be the same for forward and reverse. directions of these transitions.

With the induced (forced) nature of elementary transitions between microstates, the probability of a system transition from one region of the phase space to another is determined not only by the length of the monitoring time for this system, but also by the number of individual actions. of corresponding quantum transitions that take place in a given time interval.

– The existence of properly organized closed physical systems is assumed, for each of which the most probable (equilibrium) macroscopic state is realized with unequal probability of being in various available microstates. This may be due, for example, to a certain relationship between the angular direction of movement of quantum gas particles contained in such a system and the probability of inducing individual events of quantum transitions from one selected group of microstates of the system to another group they.

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