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A MATHEMATICAL APPROACH TO FOUNDATIONS OF STATISTICAL MECHANICS[1]

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The last quarter of this century was a time of a very intensive development of interaction between statistical mechanics and probability theory. What principally new added this development to the methodology of statistical mechanics? I think that it is possible to single out the following contributions:

1) Mathematically rigorous methods were introduced in the realm of statistical mechanics. (Of course, I understand that at least not all modern physicists agree that this contribution is a positive one.)

2) It turned out that even any real system contains a finite number of particles the mathematical laws of statistical mechanics find more explicit and transparent formulations as properties of systems with infinite number of particles. The infinity is a better approximation to the number $6 \cdot 10^{23}$ than the number 100 ($100 \ll 6 \cdot 10^{23} \approx \infty$). The number $6 \cdot 10^{23}$ is the famous Avogadro number corresponding to the number of particles in a typical macroscopic system of particles and 100 is a number of components so large that the most part of mathematical algorithms and descriptions that are applicable theoretically to any system with a finite numbers of elements becomes practically non applicable to the finite systems with such number of components.

3) Many laws of statistical mechanics are traditionally formulated as approximately valid in some situations which are not described exactly enough. It turned out that they can be treated mathematically as exact results of some well-defined limit approaches.

4)The mathematical models of statistical mechanics lost their exclusiveness. It turned out that similar models can arise in many other sciences, in situations which are far from the physical specifics of statistical mechanics. Now we have series of similar mathematical models which are equal in rights from the pure mathematical point of view and only some of them have a direct physical interpretation. It creates a possibility of wide generalizations and extends the class of more simple mathematical models that can be studied without a care on their physical reality in a hope that results can help to orient in the real physical situations.

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[1]An enlarged and revised variant of lectures given at the International Symposium in Honour of Boltzmann's 150-th birthday, Vienna, February 1994 and Boltzmann's Legacy, 150 Years after his Birth, International Conference, Rome, May 1994

The aim of this lecture is to discuss from these positions the classical problem of foundations of statistical mechanics. We concentrate on the following question. Why are the properties of the system of statistical mechanics in equilibrium can be described by Gibbsian probability distributions (the Gibbs postulate)?

Any mathematical construction has to have a starting point. Our starting point is the hypothesis that the time evolution is defined by the laws of classical mechanics. So we completely avoid possibilities and difficulties created by the quantum mechanics approach. Also we confine ourselves to consideration of systems with deterministic dynamics, where only initial realizations can be random even the problems discussed below can be formulated also for random dynamics and in such modified variant seem to be easier for an investigation. There is a voluminous mathematical literature on random dynamics of multicomponent system and in the limits of this lecture it is possible only to give a reference to excellent books of Liggett [Li] and Spohn [Sp] and the bibliography in these books. Besides it, it seems that a hope to justify the postulates of statistical mechanics in the framework of deterministic approach is important as an end in itself.

We assume that at some initial instant $t = 0$ we have a system of a large number of similar particles having a general enough statistical properties of their positions and velocities. We ask how these statistical properties will be transformed after the mechanical evolution of this system during a long enough time period t and if there is a hope to justify the statement that asymptotically, as $t \to \infty$, a Gibbsian distribution arises. Of course, it has to be the Gibbsian distribution described by the same Hamiltonian which governs the mechanical motion of the particles.

So we assume that realizations of the system of N particles at any given instant are vectors $a = (q_1, v_1, q_2, v_2, \dots, q_N, v_N)$, where the positions of particles q_i and their velocities v_i are d-dimensional vectors: $q_i, v_i \in \mathbb{R}^d, i = 1, 2, \dots, N$. We denote the space of such vectors by $\widehat{\mathcal{A}}_N$. Although the main physical case is the case $d = 3$, we want to compare the situations in different dimensions and so assume that d is an arbitrary positive integer. We assume that a potential $U(q), q \in \mathbb{R}^d$, such that $U(q) = U(-q)$ is fixed. This potential will be called the potential of dynamics. We consider the Hamiltonian dynamics governed by the Hamiltonian

$$H(a) = \frac{1}{2}\sum_{i=1}^{N} |v_i|^2 + \sum_{i<j} U(q_i - q_j), \quad a \in \widehat{\mathcal{A}}_N. \tag{1}$$

(So we suppose that the masses of the particles are equal to 1.) If U is a smooth function, the standard theorems of the theory of differential equations prove the existence and the uniqueness of the solution of the appropriate system of differential equation and so for any initial condition $a(0) \in \widehat{\mathcal{A}}_N$ a trajectory $a(t) \in \widehat{\mathcal{A}}_N, 0 \leq t < \infty$, is well defined. The system of transformations $T_t : a(0) \to a(t), 0 \leq t \leq \infty$, defines a dynamical system for which the Lebesgue measure in the $2dN$-dimensional space of realizations $a \in \widehat{\mathcal{A}}_N$ is an invariant measure (the Lioville theorem). The usual mechanical laws of conservation hold. The following two laws are important for us. One of them is the law of conservation of energy, which states that

$$H(a(t)) = \text{const}, \quad 0 \leq t < \infty. \tag{2}$$

The other one is the law of conservation of moment, which states that

$$M(a(t)) = \text{const}, \quad 0 \le t < \infty, \tag{3}$$

where the moment

$$M(a) = \sum_{i=1}^{N} v_i. \tag{4}$$

The hypothesis about a smoothness of the potential of dynamics U is too restrictive, since it is natural to suppose that particles repulse strongly at small distances and so $U(q) \to \infty$, as $q \to 0$. But in this case the law of conservation of energy does not permit collisions of particles and so, if the potential is smooth out of the point $q = 0$, we again have the statements about the existence and the uniqueness of the dynamics and about the existence of the invariant measure and the laws of conservation. Sometimes it is assumed that the particles have hard cores of a diameter $R > 0$. It means that only realizations a with $|q_i - q_j| \ge R, i \ne j, i, j = 1, 2, \dots, N$, are possible what is interpreted as the condition

$$U(q) = \infty, \quad \text{if } |q| < R. \tag{5}$$

If we assume additionally that the potential of dynamics U is smooth in the domain $|q| > R$ and $U(q) \to \infty$, as $|q| \to R$, then the trajectories are well defined and again the laws of conservation hold and the Lebesgue measure is invariant. The situation becomes more complex if the condition $U(q) \to \infty$ as $|q| \to R$ is not fulfilled as, for example, in the case of the hard spheres system, defined by the potential

$$U(q) = \begin{cases} \infty, & \text{if } |q| < b, \\ 0, & \text{if } |q| \ge b. \end{cases} \tag{6}$$

In such cases it is necessary to supplement the definition of the trajectories by a description of their behavior at instants of collisions of particles, i.e., at instants t, when $|q_i(t) - q_j(t)| = b$ for some $i \ne j$. Usually it is assumed that these collisions are elastic, since it do not violate the laws of conservation (2) and (3). But there are no natural way to continue a trajectory at the instants, when three or more particles collide. A hope is that it can occur only for some set of initial conditions of zero invariant measure.

The existence of dynamics is trivial for the case of the ideal gas, when the potential of dynamics

$$U(q) = 0, \quad q \in \mathbb{R}^d. \tag{7}$$

Then the trajectories of positions of particles are direct lines and the velocities are constant.

Models of finite systems of particles moving in all d-dimensional space does not seem promising for an asymptotical study. In typical cases the positions of all particles tend to infinity, as $t \to \infty$. So it usually assumed that particles moves inside a finite domain Ω, the volume of which $|\Omega|$ is proportional to N. It means that the trajectories take the values in the set of realizations $\widehat{\mathcal{A}}_N(\Omega) = \{a \in \widehat{\mathcal{A}}_N : q_i \in \Omega, i = 1, 2, \dots, N\}$. Then we need to supplement the definition of trajectories and to describe the law of their collision with the walls of the volume Ω. Usually it is assumed that the particles reflect elastically from the walls. In the case of the potential (6) and $d \geq 2$ a billiard terminology is often used. The volume Ω is a billiard and the particles are billiard balls. In the case of the potential (6) and $d = 1$ the system of particles is called a hard rods system. There are some difficulties with an exact mathematical definition of trajectories especially if the boundary of the domain Ω is not smooth (for example a square billiard). For the case of billiard systems the problem of the existence and uniqueness was studied in details in the book [CFS, chapter 6]. But there is an additional difficulty. An elastic reflection from a wall conserves the energy of a particle but changes its velocity. So the law of conservation of energy is fulfilled, but the law of conservation of the moment fails. However, as it is clear from the discussion below the law of conservation of moment is inherent in the very nature of the Gibbs postulate. In the framework of finite-particle approach the only possibility to save this law is to consider periodical boundary conditions, i.e., to assume that the volume in which the particles move is a torus. But it seems that this brave hypothesis is not closer to the physical reality than the hypothesis that there is an infinite system of particles used in the following.

We construct the infinite-particle dynamics as a limit of dynamics of the N particles as $N \to \infty$. To do this a little another point of view on realizations of finite particle systems is convenient. Since all the particles are similar we can make a factorization of the space $\widehat{\mathcal{A}}_N$, identifying the realizations which are obtained one from another by a renumeration of particles. Then we obtain a set of realizations that are finite subsets of the space $\mathbb{R}^d \times \mathbb{R}^d$ containing N points. We denote this set by $\mathcal{A}_N$. The definition of dynamics and its properties described above are easily extended to this situation. The space $\mathcal{A}$ of infinite system of particles is the space of all countable subsets of the space $\mathbb{R}^d \times \mathbb{R}^d$, which are locally finite in the sense that for any open cube $\Lambda_n = \{q = (q_1, q_2, \dots, q_d) : -n < q_i < n, i = 1, 2, \dots, N\}$ the subset $a|_{\Lambda_n}$ of a set $a \in \mathcal{A}$ consisting of all points from a which positions located inside Λ_n is finite. There is a natural topology in the space $\mathcal{A}$: a sequence $a_m \in \mathcal{A}$ converges to a realization a if and only if for any n the number of points in the set $a_m|_{\Lambda_n}$ coincides with the number of points in the set $a|_{\Lambda_n}$ for all large enough m and the set $a_m|_{\Lambda_n} \to a|_{\Lambda_n}$ in the natural sense. We say that for some realization $a \in \mathcal{A}$ the infinite-particle dynamics is defined if for any $t > 0$ the limit

$$T_t a = \lim_{n \to \infty} T_t(a|_{\Lambda_n}) \tag{8}$$

exists, where $T_t(a|_{\Lambda_n})$ is the realization at the instant t generated by the finite-particle dynamics in the infinite volume of particles with the initial configuration $a|_{\Lambda_n}$. It would be too much to expect that the limit (8) exists for any initial condition a. There are simple examples of situations such that at some fixed instant $t_0 > 0$ the velocity of a particle or the number of particles in a finite subvolume tend to infinity as $n \to \infty$ and so there are no natural way to prolong the infinite-particle dynamics after the instant t_0. Such collapse can occur since even for the typical initial configuration the energy of its restriction to any finite subvolume is finite its total energy is typically infinite and it can happen that this energy from infinity gathers in a finite volume after a finite period of time. So the following statement of the problem seems to be natural: to describe a sufficiently wide class of initial realizations a for which the limits (8) exist. It is possible to say a little more explicitly what means a wide enough class of realizations in this context. This class has to be so wide that it has probability 1 with respect to a wide class of probability distributions on the space of infinite realizations (this class of distributions has to include Gibbsian distributions – see below – described by a general class of potentials). The study of this problem was initiated by Lanford [La] for the case of the dimension 1 and a smooth potential and then extended to some natural classes of potentials with a repulsion at close distances and to the case $d = 2$ in the papers of Dobrushin and Fritz [DF], [FD], [F]. Restrictions on initial configurations used in these papers are explicitly described as certain restrictions on the growth of velocities and density at infinity. There are no analogous result for the most important case $d = 3$, where additional mathematical difficulties arises. It seems that for this case there is a slight hope to find mild restrictions on initial configuration which will guarantee the existence of infinite particle dynamics in an explicit way, but it is possible to hope that the dynamics exists for almost all initial configurations with respect to a wide class of initial probability measures. It is a challenging open mathematical problem. Nevertheless, we will formulate the following hypothesis in terms of infinite-particle dynamics since their reformulations in terms of finite-particle dynamics are essentially more tremendous (see a discussion in the end of the lecture). The construction of infinite particle dynamics of the ideal gas is a trivial problem and by the help of a non-linear transformation its construction for the one-dimensional hard rods system can be reduced to the case of ideal gas dynamics (see [DS]).

The main laws of conservation can be extend to the situation of infinite-particle dynamics, although, of course, their formulations need a modification. Let $\Phi = (\phi_1, \phi_2)$ be a pair of function $\phi_1(q, v)$ and $\phi_2(q_1, v_1, q_2, v_2)$. For any realization $a \in \mathcal{A}$ the limit

$$(9) \quad \overline{\Phi}(a) = \lim_{n\to\infty} \frac{1}{|\Lambda_n|}\left(\sum_{(q,v)\in a|_{\Lambda_n}} \phi_1(q, v) + \sum_{(q_1,v_1),(q_2,v_2)\in a|_{\Lambda_n}} \phi_2(q_1, v_1, q_2, v_2)\right),$$

where $|\Lambda_n|$ is the volume of the cube Λ_n, is called the density of the two-particle additive functional with the foundation Φ on the realization a (if, of course, this limit exists). We say that a law of conservation for the functional Φ and an initial realization a is fulfilled if the value $\overline{\Phi}(a(t))$ is defined for all $0 \le t < \infty$ and

$$(10) \qquad \overline{\Phi}(a(t)) = \text{const}, \quad 0 \le t \le \infty.$$

In a similar way laws of conservations for k-particle functionals can be defined. The law of conservation of moment is defined by the foundation

$$(11) \qquad \phi_1(q, v) = v, \quad \phi_2(q_1, v_1, q_2, v_2) \equiv 0.$$

The corresponding density is denoted by $\overline{M}(a)$. The law of conservation of energy is defined by the foundation

$$(12) \qquad \phi_1(q, v) = \frac{1}{2}|v|^2, \quad \phi_2(q_1, v_1, q_2, v_2) = U(q_1 - q_2).$$

The corresponding density is denoted by $\overline{E}(a)$. To this list it is necessary to add the law of conservation of the number of particles, which was trivial in the case of finite-particle dynamics. It is defined by the foundation

$$\phi_1(q,v) \equiv 1, \quad \phi_2(q_1,v_1,q_2,v_2) \equiv 0. \tag{13}$$

The corresponding density is denoted by $\overline{N}(a)$. In all the cases, when the infinite-particle dynamics is constructed, these three main laws of conservation are fulfilled with the probability 1 for a wide class of initial distributions (including the Gibbsian distributions).

We denote by $\mathcal{A}_0$ the set of all realizations $a \in \mathcal{A}$ for which the limit (8) exists for all $t \geq 0$. Then a semigroup of transformations $T_t : a \in \mathcal{A}_0 \to \mathcal{A}_0, 0 \leq t < \infty$, is defined. There is a natural Borel (with respect to the topology described above) σ-algebra of measurable subsets of the space $\mathcal{A}$. The set $\mathcal{A}_0$ is measurable and the transformations T_t are measurable transformations. Consider a state P_0, i.e., a probability measure on the space $\mathcal{A}$, such that the probability

$$P_0(\mathcal{A}_0) = 1. \tag{14}$$

Then the family of states $P_t, 0 \leq t < \infty$, is well defined by the relation

$$P_t(A) = P_0(\{a : T_t a \in A\}) \tag{15}$$

for any measurable set $A \subset \mathcal{A}$. The family P_t is called the evolution of the initial state P_0. We can formulate the Gibbs postulate as the statement that for a wide class of initial states P_0 the state P_t tends to one of Gibbsian states corresponding to the potential U governing the dynamics of the system. In all cases, when we speak about convergence of states we speak about their weak convergence with respect to the topology in the space $\mathcal{A}$ introduced above. Roughly speaking it means that the restrictions of the states to any finite volume converge in the usual weak sense and there are no requirements on uniformity of convergence in different finite volumes.

Now it is the time to recall the definition of the Gibbsian states of infinite systems of particles. To avoid some additional stipulations we suppose that the potential $U(q)$ satisfies the hard core condition (5) and vanishes out of a sphere of a radius r. Fix the parameters $\beta \geq 0$ (the inverse temperature), $\bar{v} \in \mathbb{R}^d$ (the mean velocity), and the number of particles N. The (small canonical) Gibbsian distribution in the volume Ω is a probability measure on the set $\widehat{\mathcal{A}}_N(\Omega)$ defined by the following density with respect to the usual Lebesgue measure on this set

$$p_N(a) = \frac{\exp\left\{-\beta\left(\sum_{i<j} U(|q_i - q_j|) + \frac{1}{2}\sum_i |v_i - \bar{v}|^2\right)\right\}}{Z_N(\Omega)}, \quad a \in \widehat{\mathcal{A}}_N(\Omega), \tag{16}$$

where the partition function

$$\begin{aligned} &Z_N(\Omega) \\ &= \int_{\widehat{\mathcal{A}}_N(\Omega)} \exp\left\{-\beta\left(\sum_{i<j} U(|q_i - q_j|) + \frac{1}{2}\sum_i |v_i - \bar{v}|^2\right)\right\} dq_1 \dots dq_d dv_1 \dots dv_d. \end{aligned} \tag{17}$$

So, the velocities v_i are mutually independent and have Gaussian (= Maxwell) distributions with the mean value $\bar{v}$. To define the grand canonical Gibbs distribution with a random number of particles we introduce an additional parameters $\mu \in \mathbb{R}^1$ (the chemical potential) and let $\widehat{\mathcal{A}}(\Omega) = \cup_{N=0}^{\infty} \widehat{\mathcal{A}}_N(\Omega)$. (Here $\widehat{\mathcal{A}}_0(\Omega)$ is the space consisting from one point $\emptyset$ corresponding to the empty realization.) We introduce the (Poisson) probabilities

$$P(\widehat{\mathcal{A}}_N(\Omega)) = \frac{e^{\beta\mu N}|\Omega|^N \exp\left\{-e^{\beta\mu}|\Omega|\right\}}{N!}. \tag{18}$$

The grand canonical Gibbsian distribution with parameters $\beta, \mu, \bar{v}$ is the probability measure on the space $\widehat{\mathcal{A}}(\Omega)$ such that the probability of the event $\widehat{\mathcal{A}}_N(\Omega)$ is given by (18) and that the conditional distribution of N particles under the condition $\widehat{\mathcal{A}}_N(\Omega)$ is given by (16). To define Gibbsian distribution in all the space $\mathbb{R}^d$ we need to consider a sequence of domains Ω_n tending to infinity (in the sense that any finite domain lies inside Ω_n for all sufficiently large n) and a sequence of functions $W_n(q), q \in \Omega_n$, such that $W_n(q)$ vanishes for the points q situated on a distance more than r from the boundary of Ω_n. This function will be called the boundary potential. We let

$$H_{W_n}(a) = H(a) + \sum_{i=1}^{N} W_n(q_i) \tag{19}$$

Repeating the previous construction with H changed to H_{W_n} we define the grand canonical Gibbsian distribution in the volume Ω_n with parameters $\beta, \mu, \bar{v}$ and the boundary potential W_n . Renumarating the particles and assuming that there are no particles out of Ω_n we can interpret the introduced Gibbsian distribution as a probability measure in the space $\mathcal{A}$. We say that a probability measure in the space $\mathcal{A}$ is a Gibbsian state with the potential U and the parameters $\beta, \mu, \bar{v}$ if it is a limit of Gibbsian measures with the same parameters in volumes Ω_n with the boundary potentials W_n for some sequences Ω_n, W_n or if it belongs to the closure of the set of convex linear combinations of such limits. It is well known that a Gibbsian state exists for all values of parameters $\beta, \mu, \bar{v}$ and that it is unique if the chemical potential $\mu \le \mu_0$, where μ_0 is an appropriate number (the case of rarefied gas) or if the dimension $d = 1$ (see [D2] for example). It is expected that if the dimension $d > 1$ then for large enough μ the Gibbsian state can be non-unique (a phase transition) but (unlike with the case of lattice gas models) there are no examples in which this nonuniqueness is proven in a mathematically rigorous way. So, in the following discussion we restrict ourselves to the situations, when the Gibbsian state with the given values of parameters $\mu, \beta, \bar{v}$ and the dynamics potential U is unique.

For any Gibbsian state in the domain of uniqueness the values of densities $\overline{E}(a), \overline{M}(a)$, and $\overline{N}(a)$ take values which are independent of a for almost all a (the law of large numbers). So, we can define the values $N(P), M(P), E(P)$ corresponding to a Gibbs state P. It turns out that the correspondence between triples $(\mu, \beta, \bar{v})$ and $(N(P), E(P), M(P))$ is an one-to-one correspondence. The values $M(P) = \bar{v}$, but the correspondence between pairs (μ, β) and $(N(P), E(P))$ is not given by explicit analytical formulas. (We need to make a reservation: the mentioned one-to-one correspondence is proven in a part of uniqueness domain only).

A study of an asymptotical behavior of a dynamics is natural to begin with a description of stationary points of the dynamics. We say that a state P_0 is a time-stationary state for the evolution defined by a potential U if $P_0(A_0) = 1$ and

$$P_t \equiv P_0, \quad 0 \leq t < \infty. \tag{20}$$

So the result of Marchioro, Presutti, and Pulverenti [MPP], who proved that for a wide class of potentials U any Gibbs state with this potential is time-invariant for the evolution defined by this potential, seems important. (See also the earlier papers of Sinai [Si2, Si3], who initiated a study of this problem for one-dimensional case, and the paper [PPT]). After it a question arises immediately. Do the Gibbsian states exhaust all the class of time-invariant states? In such general formulation the answer to this question is negative. It is easy to invent simple counterexamples. But there are some other natural conditions which have to be fulfilled for states pretending to be candidates for equilibrium states of statistical mechanics.

I) These states have to be invariant with respect to the space shifts in the Euclidean space of coordinates q.

II) These states have to satisfy some conditions of an asymptotic decay of correlations on large distances. Such conditions means, roughly speaking, that for functions ϕ_{V_1}, ϕ_{V_2} depending on the restrictions of realizations to finite volumes V_1, V_2 the differences of mean values

$$\langle \phi_{V_1} \phi_{V_2} \rangle - \langle \phi_{V_1} \rangle \langle \phi_{V_2} \rangle \tag{21}$$

are small, when the sets V_1, V_2 are far enough one from another. The conditions of such type are called mixing conditions in the theory of probability and can be formulated in many variants.

III) The restrictions of these states to the finite volumes must have densities and, if it is useful, it is possible to impose the smoothness conditions and other similar conditions of general type on these densities.

Conjecture I. *For a wide class of potentials U of dynamics any state which is invariant with respect to the evolution and satisfies conditions of the types I), II), III) is one of Gibbsian states with the potential U.*

This Conjecture seems to be plausible and important and, on the other hand, difficult for a proof.

An important argument in behalf of the last conjecture gives the result which was obtained in the series of papers of Gurevich, Sinai and Suhov ([GSS], [GS],[Gu]). They applied an equivalent description of an evolution of a system in terms of the usually used in statistical mechanics infinite BBGKY-system of differential equations for the multipartical correlation functions of the state P_t. (We need to mention that this equivalency for the case of infinite-particle systems was never discussed at a mathematically rigorous level at the literature.) They defined the time-invariant states as states such that their multiparticle correlation functions give a time-invariant solution of the BBGKY-system of equations. Further, they supposed a priori that the considered candidates for time-invariants states are Gibbsian states with some restrictions of a general type on the potentials describing these states. They proved that in this class of candidates only the Gibbsian states with the potential U which defines the dynamics give time-invariant solutions of the BBGKY-system. It is possible to show that any state which satisfies some strong conditions of decay of correlations is a Gibbsian state with some potentials (see [Ko]). So the a priori condition that the states are Gibbsian can be treated as a special strong variant of the conditions II), III) introduced above. In the derivation of the described results about time-invariant states the following step turns out to be the decisive one. It is proved that in some sense there are no other laws of conservation defined by additive functionals except the laws of conservation of the number of particles, of the moment and of the energy and their linear combinations.

Conjecture II. *Let a state P_0 satisfying the conditions I), II), III) introduced above is such that the mean values $N(P_0), M(P_0), E(P_0)$ are defined and there exists an unique Gibbsian state $\overline{P}$ with the potential U such that*

$$N(\overline{P}) = N(P_0), \quad M(\overline{P}) = M(P_0), \quad E(\overline{P}) = E(P_0). \tag{22}$$

Then for a wide class of potentials of dynamics the evolution $P_t, 0 \leq t \leq \infty$, with the initial state P_0 is such that

$$\lim_{t \to \infty} P_t = \overline{P}. \tag{23}$$

The Conjecture II is much stronger than Conjecture I and so seems even more difficult for a proof. There are no cases in which it is proved but if a result of a such type would be proved it could explain at a mathematical level the role which Gibbsian distributions play in the equilibrium statistical mechanics.

Some exceptional potentials of dynamics are known for which Conjectures I and II are not valid in their original formulation. They are the potential of the ideal gas (7), the potential of one-dimensional hard rods (6) and in the case of the dimension $d = 1$ the potentials

$$U(x) = cx^{-2}, \quad U(x) = \frac{a}{(sinh(br))^2}, \tag{24}$$

where $a > 0, b > 0, c > 0$. In these cases there are additional additive laws of conservations. In the ideal gas motion the particles conserve their velocities. In the hard rods motion the particles exchange their velocities in their collisions. It implies that the laws of conservations (10) are valid for the additive functionals with the foundations $\Phi = (\phi_1, \phi_2)$ such that

$$\phi_1(q, v) = \phi(v), \quad \phi_2(q, v) \equiv 0, \tag{25}$$

where $\phi(v)$ is an arbitrary function. Because of it a wider family of time-stationary states exists for these degenerate motion potentials. It is the family of states for which the positions have the Gibbsian distributions with the potential of dynamics, velocities of particles are again statistically independent of the positions of all particles and statistically independent for different particles, the probability distributions of velocities of all particles are identical, but unlike to the generic case this general probability distribution F of velocities is not obligatory Gaussian and can be arbitrary. We say that such state is Gibbsian with the probability distribution F for velocities. An analog of Conjecture I can be proved for these cases: all states which are invariant with respect to the evolution and satisfy the conditions I), II), III) (in one of their natural and wide concrete interpretation) are Gibbsian with a distribution F for velocities (see [DS]). The following statement is a natural analog of Conjecture II. Assume that an initial state P_0 satisfies the conditions I), II), III) and is such that for some probability distribution F on $\mathbb{R}^d$ for almost all with respect to this state realizations a and any measurable set $B \subset \mathbb{R}^d$ the density $\overline{\Phi}_B(a)$ of the additive functional with the foundation $\Phi_B = (\chi_B, 0)$, where χ_B is the indicator function of the set of realizations (q, v) such that $v \in B$, exists and is equal to $F(B)$. Then P_t converges to the Gibbsian state $\overline{P}$ with the probability distribution F of velocities such that $N(\overline{P}) = N(P_0)$. This statement have been also proved (see again [DS]). It seems that it an essential argument in the behalf of Conjectures I and II in the original formulation. In the case of the potentials (24) the additional laws of conservation arise from the integrability of the corresponding equations of motions and are more complex but again additional states invariant with respect to the evolution arise (see [C]).

The condition I) of space invariance of the initial state P_0 is not mandatory for Conjecture II. It can be changed on the condition that this state P_0 is spatially periodic or that it is only locally distinct from a space invariant state P_0'. The latest condition means that for a sequence of cubes Λ_n the restrictions of the states P_0 and P_0' on the complement to Λ_n asymptotically coincide (in some sense) as $n \to \infty$. A special class of states which are locally distinct from a space invariant state arises, if we consider the states, which are absolutely continuous (i.e. defined by a density) with respect to a space invariant Gibbsian state with the dynamics potential. For the last class of initial states Conjecture II is close to another conjecture which has an elegant mathematical formulation and so is popular in the mathematical literature. It is the conjecture that the dynamical system with an time-invariant and space-invariant Gibbsian measure defined by the group of transformations T_t is ergodic (= metrically transitive) or, what is stronger, this dynamical system is mixing. The mixing means that the mutual distribution of the realizations of the system in instants 0 and t defined by this dynamical system tends asymptotically, as $t \to \infty$, to the direct product $P_0 \times P_0$, i.e., realizations of the system at instances 0 and t became almost independent. This last conjecture is again a difficult open problem for the generic case and is proved for the case of ideal gas and one-dimensional hard rods system. For the case of ideal gas this conjecture is an evident implication of an old general probabilistic result [D1]. Its formulation on the language of the theory of dynamical system is due to Volkovissky and Sinai [VS], who proved also that this ideal gas dynamical system has the K-property. The references to the further papers can be found in the last review section of the paper [DS].

A traditional doubt exists. The entropy of a state P having the density $p(a)$ with respect to the Lebesgue measure is defined as

$$S(P) = -\int p(a) \ln p(a) da. \tag{26}$$

It follows from the Lioville theorem that in the case of dynamics in a finite volume $S(P_t)$ is constant in t. For a state P in the infinite volume the entropy can be defined as

$$S(P) = \lim_{n\to\infty} \frac{S(P|_{\Lambda_n})}{|\Lambda_n|}, \tag{27}$$

where $P|_{\Lambda_n}$ is the projection of the measure P to the cube Λ_n, i.e., the measure such that for any measurable set A of realizations in Λ_n the value

$$P|_{\Lambda_n}(A) = P(a : a|_{\Lambda_n} \in A). \tag{28}$$

In the general class of cases, when the existence of infinite-particle dynamics is proved, and for a wide class of space invariant initial states P_0 it is possible to prove that the entropy $S(P_t)$ exists for all t and is constant in t. Nevertheless, in the generic situation the entropy of the limit Gibbsian state

$$S(\overline{P}) > S(P_0). \tag{29}$$

Of course, it does not contradicts to Conjecture II. The mathematical explanation is simple. The entropy defined by the relation (27) is not a continuous functional on the space of states with the topology of weak convergence, it is only semicontinuous functional and so the convergence $P_t \to \overline{P}$ does not imply that $S(P_t) \to S(\overline{P})$. It is possible to give a "more physical" explanation of this effect. Entropy is a measure of dependency of positions and velocities of particles. If an initial state P_0 satisfies some conditions of decay of correlation, at the initial instant this dependence is mainly the dependence of particles which are close one to another. This dependence conserved in time but, typically, dependent particles will be far one from another for large t. Entropy does not feel it since in the definition (27) the cubes of any size are used. The topology of weak convergence means that the limit approach is taken in any finite volume separately and so this dependence is lost in the limit state. On the example of the ideal gas this mechanism is discussed in detail in the paper [DS].

There is another popular approach which is founded on the Ergodic Hypothesis which attracts by its elegant and simple mathematical formulation. Consider the dynamics T_t of the system of N particles defined by a dynamic potential U in a finite volume $\Omega \subset \mathbb{R}^d$ with elastic reflections from its walls or in a torus Ω . Let $\mathcal{A}_{N,E}(\Omega)$ be the set of all realizations a of N particles in the volume Ω such that the energy $H(a) = E$ (in the case of dynamics in a torus the additional restriction $M(a) = 0$ is added). Under mild restrictions on U and E this set is a piece of a smooth surface in an Euclidean space and so a probability measure on $\mathcal{A}_{N,E}(\Omega)$ can be defined as the limit of the normalized Lebesgue measures in the layers $\bigcup_{E':E\le E'\le E+\Delta} \mathcal{A}_{N,E'}(\Omega)$ as $\Delta \to 0$. This probability distribution is called the microcanonical Gibbsian distribution in the volume Ω and we denote it by $\mu_{\Omega,N,E}$. It follows from the Lioville theorem and the laws of conservation that this microcanonical distribution is invariant with respect to the dynamics. Assume that the volumes $|\Omega|$, the numbers of particles $N(\Omega)$, and the energies $E(\Omega)$ in these volumes tend to infinity in such a way that the finite non-vanishing limits

$$\overline{N} = \lim_{|\Omega|\to\infty} \frac{N(\Omega)}{|\Omega|}, \quad \overline{E} = \lim_{|\Omega|\to\infty} \frac{E(\Omega)}{|\Omega|} \tag{30}$$

exist. Under some additional conditions of a general type it is possible to prove that in the limit approach (30) the microcanonical Gibbsian distribution converges to a Gibbsian distribution in $\mathbb{R}^d$ defined by the dynamic potential U. It is the Gibbsian distribution P with the parameters μ, β defined by the conditions $N(P) = \overline{N}$, $E(P) = \overline{E}$ and $\bar{v} = 0$. (See results of such type in [DT], [Ge1], [Ge2], [H], [LPS1], [LPS2]).

So, it seems natural to assume that an justification of the statement that the microcanonical distribution describes the equilibrium distribution of the system of particles could be a decisive step toward the justification of statistical mechanics. Other time-invariant probability distribution could compete with the microcanonical distribution for the position to be the equilibrium distribution. The Ergodic Hypothesis mainly excludes this possibility. It states that in the class of probability distribution absolutely continuous with respect to the microcanonical distribution there are no other distributions invariant with respect to the dynamics. So it possible to compare the Ergodic Hypothesis with Conjecture I for infinite-particle systems formulated above and the a priori condition of absolute continuity with the condition III of this conjecture.

The famous Von Neumann – Birkhoff ergodic theorem is an analog of Conjecture II for the infinite-particle system. It states [B] that, if (for a given Ω, U, N and E) the ergodic theorem is valid, then for any bounded measurable function f of the realization in the volume Ω

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T f(S_t(a))\, dt = \int_{\mathcal{A}_{N,E}(\Omega)} f(a) \mu_{\Omega,N,E}(da) \tag{31}$$

in the sense of the convergence with the probability 1 with respect to the measure defined by the evolution with the initial distribution $\mu_{\Omega,N,E}$. After this result published in 1931 the Ergodic Hypothesis began to be treated as the main road to the foundation of statistical mechanics (See, for example, Khinchin book [Kh] which was the first mathematically rigorous book on statistical mechanics.) But during the next 30 years there was no progress in the proof of the Ergodic Hypothesis.

A pioneer paper of Sinai [Si1] generated an exciting hope to prove the Ergodic Hypothesis for the case of the hard sphere potential (6) on tori. A new deep branch of the theory of dynamical systems – theory of billiards was created (see the review paper of Szasz [Sz]). But the Ergodic Hypothesis turned out to be very difficult in the case of hard spheres also. After other 30 years of efforts of many scientists the best record is now the proof of Ergodic Hypothesis in the dimension $d = 2$ for $N = 3$ balls and in the dimension $d = 3$ for $N = 4$ balls (see Bunimovich, Sinai [BS] for $N = 2, d = 2$, Sinai, Chernov [SC] for $N = 2, d \geq 2$, Kramli, Simanyi, Szasz [KSS1] for $N = 3, d \geq 2$ and [KSS2] for $N = 4, d \geq 3$). On the other hand there are pessimistic indications. In a paper of Markus and Meyer [MM] it is proved that in the space of smooth Hamiltonians the Hamiltonians generating nonergodic dynamical systems for a set of values of energy E of a positive measure form a dense open subset. So perspectives for a proof of the Ergodic Hypothesis in a generic situation of statistical mechanics seem very vague now.

Of course a nonfulfillment of the Ergodic Hypothesis does not undermine the foundations of statistical mechanics. Some compromise variants of this hypothesis are discussed in the literature. For example, it is possible that even the Ergodic Hypothesis is not valid and there are several ergodic components, for large N one of these components covers the main part of the phase space. Another variant seems more plausible. For large N there is a lot of small ergodic components which are intermixed in a so complex way that using an observations in a fixed subvolume we almost can not distinguish these components. It is difficult to formulate exactly such hypothesis and even more difficult to deduce its implications. Really on this way we approach to Conjectures I and II for infinite-particle systems formulated above.

There is an additional complication which arises even if the Ergodic Hypothesis is valid. The ergodic theorem does not state that the convergence in (31) is uniform in N. If we define the relaxation time $T(\epsilon)$ as the minimal value of T such that the difference between the integral in the left part of (31) normalized by the multiplier T^{-1} and its limit value smaller than ϵ it seems that the best estimate for this relaxation time which could be extracted from the constructions usually used in the proof of the ergodic theorem will grow exponentially with N. Roughly speaking, the mechanism of this construction is such that before the time $T(\epsilon)$ the trajectory need to visit a small enough neighborhood of the each point of the phase space. But the volume of the space grows exponentially with N and so the time $T(\epsilon)$ has to grow proportionally to this volume. On the other hand, the physical intuition and experience suggest that the relaxation time for a realizations in a fixed subvolume does not depend on the number of particles in the whole volume. Of course, it is possible to assume that for a fixed function f depending on a restriction of realizations to a finite subvolume only the convergence in (31) is really uniform in N but the proof of such hypothesis requires entirely another ideas.

So I am glad a possibility to cite an aphoristic words of Prof. J. Lebowitz at the Vienna International Symposium in Honor of Boltzmann's 150-th Birthday which stated that now it is the real time to recognize hat the Ergodic Hypothesis is not a necessary and is not a sufficient condition for the foundation of statistical mechanic.

Within the framework of the finite-particle approach it is also possible to formulate a conjecture avoiding difficulties connected with the Ergodic Hypothesis and the ergodic theorem discussed above. Consider the sequences of cubes Λ_n and the dynamics T_t^n for the realizations in these cubes and the corresponding microcanonical distributions $\mu_n = \mu_{\Lambda_n, N_n, E_n}$ such that $N_n/|\Lambda_n| \to \overline{N}$ and $E_n/|\Lambda_n| \to \overline{E}$ (cf. (30)). Let P be the corresponding limit Gibbsian state and f be an bounded measurable function depending on the restriction of realizations to a fixed subvolume.

Conjecture III. *The relation*

$$\lim_{n\to\infty} \lim_{T\to\infty} \frac{1}{T} \int_0^T f(T_t^n a|_{\Lambda_n})\, dt = \int_{\mathcal{A}} f(a) P(da), \tag{32}$$

where (out of prudence) *the convergence is treated as the convergence in probability, holds. The convergence in T in the inner limit is uniform in n.*

Of course, this conjecture is again a very difficult open problem. It seems that its proof will require new methods, for which in a contrast to the methods used in proofs of Ergodic Hypothesis and the ergodic theorem an increase of N does not hamper but facilitates the situation. An allusion to such possibility gives a mechanism applied in all the papers devoted to much more primitive models of the ideal gas and of the one-dimensional hard rods in the infinite volume. Here because of the condition II) about of a decay of correlation in the initial moment there is an "initial store of randomness in infinity". The moving particles spread this "store of randomness" over all the space. After a long time t the situation in a given subvolume combine the initial information from different distant parts of the space and it creates the necessary mixing. Of course, the interaction between the particles tangles and covers this picture. Nevertheless it is possible to hope that a similar mechanism works also for interacting systems, especially in the case of rarefied gas, when long periods of free motion of particles alternate with shorter periods of their interaction in small groups.

The main aim of this lecture is to attract attention of ambitious representatives of the next generation of specialists in mathematical statistical mechanics to this range of difficult but important problems.

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