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ON THE CONDITION FOR THE EXISTENCE OF THE STATIONARY DENSITY IN PHASE AND ITS CONSEQUENCES

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The properties of the stationary density in phase are studied by dividing the phase space into two parts: the bounded (P_1) and unbounded part (P_2) of the Hamiltonian. We show that the existence of the stationary density in phase is determined by the existence of the bounded motions. The stationary and normalized density in phase may not be different from zero in the unbounded part P_2 of the phase space P. We study the relevance of the condition for the existence of the stationary density in phase for the Leaf, Schieve and Davidson, Rae solutions of the problem of the approach of equilibrium in systems with Hamiltonians expressible in action angle variables.

1. Introduction

In recent investigations of the spectral properties of the Liouville operator[1-5] several important theorems have been derived. Some of them might have far reaching consequences in statistical mechanics. In particular, we emphasize the property that the bounded part P_1 of phase space P (the set of points in phase space connected with the bounded motion) is the smallest invariant set with the property that the point spectrum of L restricted to P_1 contains the zero and the point spectrum of L restricted to $P_2 = (P \setminus P_1)$ does not contain the zero.

Dedicated to the memory of Prof. Aleksandar Milojević whose interest in statistical mechanics was permanent and encouriging.

In the present article we want to elaborate further the above mentioned and similar statements from Spohn's article[1], and to study its consequences for the stationary density in phase. For this aim in Chapter 2 we show that the existence of stationary density in phase is determined by the existence of the bounded motions. In the same Chapter we show also that stationary and normalized density in phase may not be different from zero in the unbounded part P_2 of the phase space P. Similar conclusions follow from Spohn's theorems. But, Spohn's theorems are based on the spectral theory and are expressed in terms of the spectral properties of the Liouville operator, whereas density in phase and its properties are the elements of our analysis.

In Chapter 3 we investigate whether and how in the familiar canonical distribution (widely used in statistical mechanics) is incorporated the difference between the bounded and unbounded solutions of Hamilton's equations of motion. We show that the canonical distribution is stationary if and only if the subset in phase space on which is defined the initial distribution is a bounded invariant set.

In Chapter 3 we study also the relevance of the condition for the existence of the stationary density in phase for the Leaf and Schieve[14,15], Davidson and Rae[16] solution of the problem of the approach of equilibrium in systems with Hamiltonians expressible in action angle variables.

2. *Bounded and unbounded motions and the existence of the stationary density in phase*

Let's denote by $x = (\vec{q}_1 \dots \vec{q}_k \vec{p}_1 \dots \vec{p}_k)$ a point in phase space P ($\vec{q}_1$ is the set of Descartes coordinates) of the mechanical system with $N = 3k$ degrees of freedom (k is the number of particles). P is connected and open subset of R^{2N} with the $2N$-dimensional Lebesgue measure μ. The dynamics of the system is described by the solutions of Hamilton's equations of motion

$$\dot{\vec{p}}_k(t) = -\frac{\partial H}{\partial \vec{q}_k} \qquad \dot{\vec{q}}_k(t) = \frac{\partial H}{\partial \vec{p}_k} \tag{II.1}$$

where H: $P \to R$ is the (twice differentiable) Hamiltonian function of the system.

We assume that for every initial value $x_0 = (\vec{q}_{10} \dots \vec{q}_{k0}, \vec{p}_{10} \dots \vec{p}_{k0}) \in P$ there exists a unique global solution

$$t \to x(t, x_0), \qquad -\infty < t < \infty \tag{II.2}$$

of (II.1). Then the mappings

$$T_t\colon\ x_0 \to x(t, x_0) \quad t \in R^1 \tag{II.3}$$

corm a one-parameter group of canonical transformations of P onto P. We will fall a triplet (P, μ, T_t) a Hamiltonian system.

A set $\Delta \in P$ is called *invariant*, if Δ is measurable and $T_t \Delta = \Delta$ almost everywhere (a. e.) for all $t \in R^1$, and strictly invariant, if Δ is measurable and $T_t \Delta = \Delta$ for all $t \in R^1$.

It is also usefull to define the bounded and the unbounded part of the Hamiltonian system. We define the *bounded part* P_1 of the Hamiltonian system (P, μ, T_t) to be the set

$$P_1 = [x \in P | \; [T_t x | \; t \in R] \text{ is bounded}]. \tag{II.4}$$

The *unbounded part* P_2 of (P, μ, T_t) is the complement of P_1

$$P_2 = P \setminus P_1. \tag{II.5}$$

P_2 and P_1 are strictly invariant sets.

Furthermore, the bounded part P_1 can be divided into two invariant subsets defined as follows[6,7].

$$P_1' = [x \in P_1 | \; [T_t x | \; t \in R] \text{ is an open trajectory}]$$
$$P_1'' = [x \in P_1 | \; [T_t x | \; t \in R] \text{ is a closed trajectory}]. \tag{II.6}$$

The invariance of these subsets follows from the fact that the trajectory $L_x = [x(t, x)]$ is the minimal invariant subset of the dynamical system (P, μ, T_t).

We shall restrict our attention to the s. c. continuous dynamical systems, defined trough the following conditions on the trajectories:

i°) $x(t, x)$ is continuous with respect to (t, x)

ii°) $x(0, x) = x$

iii°) $x(\tau, x(t, x)) = x(t + \tau, x)$. (II.7)

The point x^0 is called the limiting point of the trajectory L_x, if $x^0 = \lim_{n \to \infty} x(t_n, x)$, $t_n \in R^1$. The set which contains all limiting points x^0 is the limiting set Ω. It is obvious that if Ω is the empty set, the trajectory L_x is homomorphous to R^1 and it forms a closed set in P.

The state of the Hamiltonian system (P, μ, T_t) is given by the function s. c. state function ϱ on P. Its time evolution is determined by[8-11]

$$\varrho(x, 0) = \varrho(T_t(x), t) \tag{II.8}$$

$$\varrho(x, t) = \varrho(x^{-1}(t, x), 0) \tag{II.8a}$$

where by $x^{-1}(t, x)$ we denote the inverse function of the function $x(t, x)$. We will call this relation the dynamical law for the density in phase.

We are dealing only with those dynamical systems for which the condition (II.7) imply the continuity of the function ϱ, also.

For Hamiltonians which are invariant under the time reversal, the solutions of Hamilton's equations have the property

$$x^{-1}(t, x) = x(-t, x). \qquad \text{(II.9)}$$

For such systems one has[9,10]

$$\varrho(x, t) = \varrho(x(-t, x), 0). \qquad \text{(II.10)}$$

If the contact with the equilibrium statistical mechanics has to be made then one interprets the state function ϱ as the probability density in which case two supplementary conditions have to be satisfied[12]

$$\varrho(x, t) > 0 \qquad \text{(II.11)}$$

$$\int_P \varrho(x, t)\,\mathrm{d}x = 1, \;\; \forall t. \qquad \text{(II.12)}$$

If follows from (II.8) and (II.1) that ϱ satisfies the differential equation

$$\frac{\mathrm{d}\varrho}{\mathrm{d}t} = \frac{\partial \varrho}{\partial t} - [H, \varrho] = 0. \qquad \text{(II.13)}$$

In particular, the stationary density in phase satisfies[10-13]

$$\frac{\partial \varrho(x, t)}{\partial t} = [H, \varrho] = 0, \quad \forall x \wedge \forall t. \qquad \text{(II.14)}$$

Now, we observe *firstly* that stationary and normalized density in phase cannot be different from zero on the subset of P_2 of non-zero measure. In fact it is shown below that on the unbounded part P_2 of the phase space P it is not possible to satisfy simultaneously the dynamical law (II.8), the normalization condition (II.12) and the stationarity condition (II.14).

Let us introduce the subset $D_0 \subset P_2$ of non-zero measure which does not contain more than one point of any trajectory from certain set of phase trajectories.

We will suppose that: a) $\varrho(x, 0)$ is different from zero on a subset D_0, b) the integral

$$\int_{D_0} \varrho(x, 0)\,\mathrm{d}x = a, \qquad a < 1 \qquad \text{(II.15)}$$

is a finite number. According to (II.3) the application of T_t on the points of D_0 results to the set D_t. The sets D_t and $D_{t'}$ have two important properties

i) $D_t \cap D_{t'} = 0, \qquad \forall (t, t')$ (II.16)

ii) $\bigcup_{t=0}^{\infty} D_t$ is an unbounded set in phase space. (II.17)

It follows from the dynamical law (II.8) for the density in phase that

$$\int_{D_t} \varrho(x, t)\, \mathrm{d}x = a, \qquad \forall t. \tag{II.18}$$

But, the stationary density in phase satisfies.

$$\varrho(x, t) = \varrho(x, 0) \quad x \in D_t, \quad \forall t. \tag{II.19}$$

Combining (II.18) and (II.19) we obtain:

$$\int_{D_t} \varrho(x, 0)\, \mathrm{d}x = a, \qquad \forall t. \tag{II.20}$$

This means that $\varrho(x, 0)$ has to be different from zero on every set D_t and that the integral of $\varrho(x, 0)$ over D_t has to have the value a, $\forall t$.

Because of the properties (II.16) and (II.17) the integral of $\varrho(x, 0)$ over phase space is infinite what means that the stationary density in phase is not normalisable in the subset P_2 of the phase space P.

Secondly, it follows from Spohn's theorems derived in $\mathscr{L}^2(P)$ space that if f is an integral of motion and the normalisable function $\varrho(x, t) = f$ has to satisfy the stationarity constraints (II.14) (the Liouville operator has the eigenvalue zero), then this function is different from zero only on an invariant subset of P_1, including P_1 itself.

3. *The relevance of the conditions for the stationary density in phase for the canonical distribution*

In the equilibrium statistical mechanics combining the probabilistic arguments (ensemble interpretation) and thermodynamical arguments (judgment by the structural analogies of functional dependences) the Gibbs canonical distribution is chosen as the solution of the Eq. (II.14)[12]

$$\varrho_{eq}(\vec{p}, \vec{q}) = \exp(-H(\vec{p}, \vec{q})/\Theta) / \int_G \exp(-H(\vec{p}, \vec{q})/\Theta)\, \mathrm{d}\vec{p}\, \mathrm{d}\vec{q}$$
$$G = [(\vec{p}, \vec{q}) |\ \vec{q} \in V, p_{ix}, p_{iy}, p_{iz} \in (-\infty, \infty)]. \tag{III.1}$$

By V is denoted certain region in three-dimensional configuration space and also the volume of this region.

It is implicitly assumed that the time dependence is expressed via the domain transformation. It may be stated:

$$\varrho(\vec{p}, \vec{q}, 0) = \exp(-H(\vec{p}, \vec{q})/\Theta) / \int_G \exp(-H(\vec{p}, \vec{q})/\Theta)\, \mathrm{d}\vec{p}\, \mathrm{d}\vec{q}, \ (\vec{p}, \vec{q}) \in G$$
$$\varrho(\vec{p}, \vec{q}, 0) = 0, \qquad (\vec{p}, \vec{q}) \notin G \tag{III.2}$$

and

$$\varrho(\vec{p}, \vec{q}, t) = \exp(-H(\vec{p}, \vec{q}))/\Theta / \int_{T_t G} \exp(-H(\vec{p}, \vec{q})/\Theta)\, d\vec{p}\, d\vec{q}, \quad (\vec{p}, \vec{q}) \in T_t G$$

$$\varrho(\vec{p}, \vec{q}, t) = 0, \quad (\vec{p}, \vec{q}) \notin T_t G. \tag{III.3}$$

The normalization condition is satisfied and the stationarity requirement demands $T_t G = G$.

Although the above consideration might appear formal and superficial its importance is seen by studying the question of the invariance of the set G defined in (III.1) and subsequently (in the next section) the relevance of the result obtained for the analysis of (non-interacting) systems approaching equilibrium state.

With respect to the problem of the invariant (sub)set in phase space we remark that if V is an arbitrary region in configuration space, and if H is a function of phase variables only, invariant sets of H are independent of V, and consequently G is not an invariant set. In this case the function (III.1) is not the solution of the Eq. (II.14).

In order to build an invariant set one has to deal with the Hamiltonian which is a function of $(\vec{p}, \vec{q})$ and of V. Let's consider the familiar case when in (III.1) the Hamiltonian $H(\vec{p}, \vec{q})$ is substituted by the new Hamiltonian

$$\mathscr{H}(\vec{p}, \vec{q}, V) = H(\vec{p}, \vec{q}) + U(\vec{p}, \vec{q}, V)$$

where

$$U(\vec{p}, \vec{q}, V) = \begin{cases} \infty & \vec{q}_i \notin V \\ 0 & \vec{q}_i \in V \end{cases} \qquad i = 1 \ldots N. \tag{III.4}$$

This particular potential causes that the Hamiltonian is not continuous and is not differentiable. Also, this potential radically changes the set of trajectories of the Hamiltonian H on the phase space P. The trajectories from the set P_2 are essentially changed. Namely, under the influence of the potential U the unbounded trajectories of H become bounded trajectories of $\mathscr{H}$. The potential operates on the trajectories from P_1 in two different ways. The trajectories of H which are inside V are not influenced by the potential U. The trajectories of H which touch or cross the boundaries of the region V are influenced and radically changed by the existence of the potential U.

Consequently if one adds the potential U to the Hamiltonian H in order to make the set $G \subset P$ invariant, one indirectly changes the mechanical model of the thermodynamical system. If the Hamiltonian H has no bound states then even from »physical reasons« it is necessary to add the »walls« of the potential. But, if Hamiltonian H has bounded trajectories, U may have different influence on different trajectories. Moreover if Hamiltonian has both bound and unbounded trajectories then evidently U has very different role in different parts of the phase space P. The above procedure, however, causes the conceptual difficulties. The essence of those new difficulties lie in the fact that the existence of two sets of trajectories of the Hamiltonian H is not at all important for the canonical distribution which serves as a basis for the thermodynamics of this mechanical model.

4. The approach of equilibrium in systems with Hamiltonians expressible in action-angle variables

We will now use the above analysis to study the time-dependent solution of the Liouville equation in the case when there exists a canonical transformation from initial variables (p, q) to action variables $(\mathcal{J}, \Phi)$ so that Hamiltonian is a function of action variables only

$$(p, q) \rightarrow (\mathcal{J}, \Phi)$$
$$H = H(\mathcal{J}_1, \mathcal{J}_2 \dots \mathcal{J}_N) = H(\mathcal{J}) \qquad \text{(III.5)}$$

In this case the solution of Hamilton's equations

$$\dot{\Phi}_i = \frac{\partial H}{\partial \mathcal{J}_i} = \omega_i(\mathcal{J}) \qquad \dot{\mathcal{J}}_i = \frac{\partial H}{\partial \Phi_i} = 0$$

reads

$$\mathcal{J}_i = \mathcal{J}_{i0} \quad \Phi_i = \omega_i(\mathcal{J}) \cdot t + \Phi_{i0}, \quad i = 1, \dots, N. \qquad \text{(III.6)}$$

Consequently, the definition property of the density in phase takes the form.

$$\varrho(\Phi, \mathcal{J}, t) = \varrho(\Phi_0 - \omega t, \mathcal{J}, 0). \qquad \text{(III.7)}$$

At the same time this is the final form of the solution of the Liouville equation.

In the simplest case of the free particle Hamiltonian

$$H = \sum_i \frac{\vec{p}_i^{\,2}}{2m} \qquad \text{(III.8)}$$

action and angle variables and frequencies are

$$\mathcal{J}_l = p_l; \; \Phi_l = q_l, \quad \omega_l(\mathcal{J}) = \frac{p_l}{m}, \quad l = 1 \dots, N \qquad \text{(III.9)}$$

whereas density in phase is given by

$$\varrho(\vec{p}, \vec{q}, t) = \varrho(\vec{p}, \vec{q} - \omega(\vec{p})\, t, 0). \qquad \text{(III.10)}$$

Recently, Leaf and Schieve[14,15], Davidson and Rae[16] investigated whether in »thermodynamical limit« the solutions (III.7) and (III.10) of the Liouville equation tend for $t \rightarrow \infty$ to a time-independent function, i. e. whether they approach the stationary solution of the Liouville equation.

In order to find the solution (III.7) of the Liouville equation they used the method which for the first time used "Prigogine[17] by noting that the Liouville equation has the same form as the Schrödinger equation. In this method the volume of the system is by definition related to the function space in which operates the Liouville operator

$$L = - \sum_{l=1}^{N} \omega_l (\mathcal{J}) \cdot \frac{\partial}{\partial \Phi_l} \qquad \text{(III.11)}$$

$$L = - \sum_{j=1}^{k} \frac{\vec{p}_j}{m} \cdot \frac{\partial}{\partial \vec{q}_j}. \qquad \text{(III.12)}$$

Consequently, the initial density in phase for V finite is periodic in $\vec{q}_l$ and for $V \to \infty$ is not periodic in $\vec{q}_l$. From $\varrho(\Phi, \mathcal{J}, t)$ written in form of the Fourier series (V finite) and Fourier integrals ($V \to \infty$) those authors concluded that $\varrho(\Phi, \mathcal{J}, t)$ does not become time independent for large t even in »thermodynamical limit«. In fact they concluded that the existence of the limit for $t \to \infty$ is independent whether V is taken to be finite or infinite.

We will now comment this conclusion on the basis of the results exposed in Sec. II.

If the Hamiltonian which is expressible in angle and action variables has no bound states (like the free particle Hamiltonian) there is no normalisable stationary density in phase and therefore it is not suprising that there is no time dependent solution tending to time-independent one.

If Hamiltonian has periodic solutions in $(\vec{p}, \vec{q})$ space, it is not hard to see that the function $\varrho(\vec{p}, \vec{q}, t)$ associated with $\varrho(\vec{p}, \vec{q}, 0)$ which is not a function of integrals of motion can not become time independent. On the other hand $\varrho(\vec{p}, \vec{q}, t)$ associated with $\varrho(\vec{p}, \vec{q}, 0)$ being a function of integrals of motion is stationary $\forall t$.

5. *Conclusions*

We have studied the properties of the stationary density in phase by dividing the phase space into two parts: the bounded (P_1) and unbounded part (P_2) of the Hamiltonian H. We argue that the existence or nonexistence of those two parts is an important and characteristic feature of the mechanical model and that this feature of the mechanical model should be preserved in the construction of the elements of the statistical theory, especially of the density in phase.

Our main result reads: »Stationary, continuous and normalized density in phase cannot be different from zero on the subset of P_2 of non-zero measure«.

We show also that this explains the result reached by Leaf and Schieve[14,15], Davidson and Rae[16] according which the density in phase corresponding to the Hamiltonian expressible in angle action variables does not become time-independent for $t \to \infty$. In the case of the free particle Hamiltonian this result is of high importance because many authors[11-13] explain the existence of the Maxwell-Boltzmann distribution in an ideal gas on the basis of the canonical distribution (III.1) arguing that it is the stationary distribution of the corresponding Liouville equation.

But this distribution has two essential shortcomings. First is related, as we showed in this article, with the fact that it is associated with the Hamiltonian which has no bound states, and consequently stationary density in phase does not exist. Therefore, it is not surpising that there is no time dependent solution tending for $t \rightarrow \infty$ to the time-independent one. Second shortcoming is related, as pointed out by Koga[19], with the fact that this distribution does not take into account the collisions between the particles, which on the other hand, according to the kinetic theory of gases are the basic mechanism of equilibration.

References

1) H. Spohn, Physica **80A** (1975) 323;
2) . Spohn, J. Math. Phys. **17** (1976) 57;
3) H. Spohn, Rep. Math. Phys. **8** (1975) 363;
4) R. T. Prosser, J. Math. Phys. **10** (1969) 2233;
5) R. T. Prosser, J. Math, Phys. **13** (1972) 186;
6) M. Henon and C. Heiles, The Astron. J. **69** (1964) 73;
7) J. Ford and G. H. Walker, Phys. Rev. **188** (1969) 416;
8) B. O. Koopman, Mathematics **17** (1931) 315;
9) A. I. Ahiezer and S. V. Peletminskij, *Metodi Statističeskoj fiziki* (Nauka, Moskva 1977);
10) O. Penrose, Rep. Prog. Phys. **42** (1979) 1937;
11) J. P. Terleckij, *Statističeskaja fizika* (Vishaja shcola, Moskva 1966);
12) W. Gibbs, *Elementary principles in statistical mechanics,* collected works, Vol. II (New Haven 1948);
13) K. Huang, *Statistical Mechanics* (John Wiley and Sons, Inc. New York 1963);
14) B. Leaf and W. Schieve, Physica **30** (1964) 1389;
15) B. Leaf and W. Schieve, Physica **36** (1967) 345;
16) R. Davidson and J. Rae, J. Phys. **A3** (1970) 128;
17) I. Prigogine, *Non Equilibrium Statistical Mechanics* (Interscience, New York 1962);
18) H. Goldstein, *Classical Mechanics* (Addison-Wesley, Reading, Massachusetts 1980);
19) T. Koga, *Introduction to Kinetic Theory* (Oxford, Pergamon Press 1970).

O USLOVU EGZISTENCIJE STACIONARNE FAZNE GUSTINE I ODGOVARAJUĆIM POSLEDICAMA

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Originalni naučni članak

Studirana su svojstva stacionarne fazne gustine deobom faznog prostora na dva dela: ograničen (P_1) i neograničen deo (P_2) Hamiltonijana. Pokazali smo da je egzistencija stacionarne fazne gustine određena egzistencijom ograničenih kretanja. Stacionarna i normalizovana fazna gustina ne može biti različita od nule u neograničenom delu P_2 faznog prostora P. Studirali smo relevantnost ovog uslova egzistencije stacionarne fazne gustine za Leaf, Schieve i Davidson, Rea rešenje problema dostizanja ravnoteže u sistemima čiji se Hamiltonijan može izraziti pomoću ugaono-akcionih varijabli.