ON SOME PROPERTIES OF NONCONSERVATIVE SYSTEMS OF CLASSICAL STATISTICAL MECHANICS

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Abstract

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ON SOME PROPERTIES OF NONCONSERVATIVE SYSTEMS OF CLASSICAL STATISTICAL MECHANICS

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In the case when the total energy of a mechanical system is not conserved in time, the system is called nonconservative. Strictly speaking, the notion of conservative mechanical systems is an idealization, all the more justified the more negligible are the losses or influxes of energy into the particular system under study over the time intervals of the evolution of interest to us. Turning to the study of nonconservative systems, we shall proceed from the idea that the exchange of energy with the environment surrounding the system occurs through the action of external forces on the motion of the particles of the system.

Let (p, q) be the aggregate of the momenta and coordinates of the particles constituting the given system. Let also $H(p, q)$ be the Hamiltonian function of the system, equal to the sum of the kinetic energy of the particles and the total potential energy of interaction of the particles with one another, as well as with the walls and any constant external field. Thus the function $H(p, q)$ includes all those terms which would have been present if there were no exchange of energy with the external medium. We denote by $G_k(p, q, t)$ the external generalized force acting on the k-th particle. Then the motion is described, in general, by the non-Hamiltonian system of equations:

$$\dot{q}_k = \partial H/\partial p_k; \qquad \dot{p}_k = -\partial H/\partial q_k + G_k(p, q, t), \quad k = 1, 2, \dots, N. \tag{1}$$

From the form of (1) it is easy to obtain a number of simple consequences.

1. Generalized Liouville equation. The velocity of the point representing the mechanical system in $6N$-dimensional phase space is written as

$$\mathbf{v} = (\dot{q}_1, \dot{q}_2, \dots, \dot{q}_N, \dot{p}_1, \dot{p}_2, \dots, \dot{p}_N).$$

Directly from equations (1) it follows that

$$\operatorname{div}\mathbf{v} = \sum_{1\le i\le N}\left(\frac{\partial \dot q_i}{\partial q_i}+\frac{\partial \dot p_i}{\partial p_i}\right)=$$

$$=\sum_{1\le i\le N}\left(\frac{\partial^2 H}{\partial p_i\partial q_i}-\frac{\partial^2 H}{\partial q_i\partial p_i}+\frac{\partial G_i}{\partial p_i}\right)=\sum_{1\le i\le N}\frac{\partial G}{\partial p_i}. \tag{2}$$

Let ρ denote the probability density of finding the mechanical system in the volume $dp_1 dp_2 \ldots dp_{Ndq} 1 dq_2 \ldots dq_N$ near the point (p, q) of phase space.

We obtain the generalized Liouville equation from the continuity condition

$$\partial\rho/\partial t + \operatorname{div}(\rho\mathbf{v}) = 0.$$

Using expression (2) for $\operatorname{div}\mathbf{v}$, it is not difficult to obtain

$$\frac{\partial\rho}{\partial t} = \{H;\rho\} - \sum_{1\le i\le N}\frac{\partial}{\partial p_i}(G_i\rho). \tag{3}$$

Here $\{H;\rho\} \equiv \sum(H'_{q_i}\rho'_{q_i} - H'_{p_i}\rho'_{p_i})$ are the usual Poisson brackets.

Remark. From the generalized Liouville equation (3) and expression (2) it is clear that the analytic criterion for nonconservativity of a mechanical system has the form $\sum \partial G_i/\partial p_i \ne 0$. In the case where the written sum is equal to zero, by a certain redefinition of the function H the system can always be made Hamiltonian.

2. Absence of integrals of motion. Let $F(\rho)$ be an arbitrary measurable function of ρ. We shall show that the integral over phase space $\int\cdots\int F\,dp\,dq$ is a function of time t.

Indeed, by a well-known consequence of Liouville' s theorem, the indicated integral is independent of time if and only if the substantial derivative of ρ is zero:

$$\frac{D\rho}{Dt} = 0, \qquad \text{where} \quad \frac{D}{Dt} = \frac{\partial}{\partial t} + \sum_{(i)}\left(\dot q_i\frac{\partial}{\partial q_i} + \dot p_i\frac{\partial}{\partial p_i}\right).$$

In the present case

$$\frac{D\rho}{Dt} = -\rho\sum_{(i)}\frac{\partial G_i}{\partial p_i} \ne 0. \tag{4}$$

Corollary. $\int\cdots\int \rho\,dp\,dq = A(t)$.

Thus the motion in phase space of the point representing a mechanical system takes place not on a constant in time, but on a continuously deforming energy surface. Of course, this fact is quite obvious even without a special proof.

3. Change of probability density under motion together with the flow of mechanical systems. Let ρ_0 be the probability density at the point $(p(t_0), q(t_0))$ at time t_0, and let $\rho^*(t)$ be the probability density at the point of phase space $(p(t), q(t))$ at time $t > t_0$, with the second point lying on the trajectory of the mechanical system which at time t_0 emerged from the point $(p(t_0), q(t_0))$. The relation between the functions ρ^* and ρ is obtained by integrating equation (4):

$$\rho^* = \rho_0 \exp\left(-\int_{t_0}^{t} \sum_{1\le i\le N} \frac{\partial G_i(\xi)}{\partial p_i}\, d\xi\right). \tag{5}$$

Let us emphasize that the functions ρ^* and ρ are taken at different points of phase space.

Corollary. Let V_0 be a certain distinguished volume occupied by part of an ensemble of mechanical systems in phase space at time t_0. Then, as follows from formula (5), at time $t > t_0$ the same part of the ensemble occupies the volume

$$V = \int_{\Omega_0} dp_0\, dq_0\, \exp\left(\int_{t_0}^{t} \sum_{1\le i\le N} \frac{\partial G_i(\xi)}{\partial p_i}\, d\xi\right). \tag{5a}$$

We note that formula (5a) was obtained by S. Guashi in work ([1]) by direct calculation of the quantity $\partial(p, q)/\partial(p_0, q_0)$. The other results of S. Guashi are erroneous.

4. Normalization. From the remark following formula (4) it is clear that the usual normalization of the function ρ is impossible: at each given instant of time the mechanical system is certainly located at some point of phase space, but energy exchange continuously changes the ensemble. Obviously, the function ρ^* must be normalized to a constant.

Set $\bar{\rho}^* = C\rho$ under the condition $\int \rho^*\, dp\, dq = 1$. The integration extends over the entire phase space. Then

$$C\int \rho^*(p, q)\, dp\, dq = C\int \rho_0(p_0, q_0) \exp\left[-\int \sum \frac{\partial G_i}{\partial p_i}\, d\xi\right] \frac{\partial(p, q)}{\partial(p_0, q_0)}\, dp_0\, dq_0 = 1.$$

A direct calculation shows that

$$\partial(p, q)/\partial(p_0, q_0) == \exp\left(\sum \int d\xi\, \partial G_i/\partial p_i\right)$$

and, consequently,

$$C = \left(\int \rho_0(p_0, q_0)\, dp_0\, dq_0 \right)^{-1}.$$

Thus, the normalized function ρ^* has the form:

$$\bar{\rho}^*(p, q, t) = \left[\rho_0(p_0, q_0, t_0) \Big/ \int \rho_0(p_0, q_0, t_0)\, dp_0\, dq_0 \right] \exp\left[-\int_{t_0}^{t} \left(\sum_{(i)} \frac{\partial G_i(\xi)}{\partial p_i} \right) d\xi \right]. \tag{6}$$

Remark. In the case $\sum \partial G_i/\partial p_i = 0$ we have $\bar{\rho}^*(t) = \rho_0(t_0)/\int \rho_0\, dp_0\, dq_0$, i.e., the probability density is conserved along the flow, which is characteristic of conservative systems.

5. Asymptotic character of ρ^*. Of course, one can cite many examples of nonconservative systems, for instance stars or microscopic particles radiating energy outside the system or absorbing radiation. Radiation leads to a change in the momenta of mechanical objects. Let us consider forces G_i of an idealized character: let energy be continuously introduced into or removed from the system by means of "friction forces" $G_i = \alpha p_i$. In the case $\alpha > 0$ energy is introduced into the system; for $\alpha < 0$ it is removed.

In the first case, any selected volume of "probability fluid" becomes infinitely large as $(t - t_0) \to \infty$, while in the second it tends to zero. At the same time

$$\lim_{(t-t_0)\to\infty} \bar{\rho}^* = \lim_{(t-t_0)\to\infty} C\rho_0 e^{-\alpha N(t-t_0)} = \begin{cases} 0 & (\alpha > 0), \\ \infty & (\alpha < 0). \end{cases}$$

This means that when energy is pumped in, the ensemble of systems spreads out in momentum–velocity space, while when energy is pumped out all systems of the ensemble flow into a neighborhood of the point $(p, q) = (0, q_0)$.

Suppose that at the moment t_0 the ensemble consisted of equilibrium systems and $(t - t_0) \to \infty$. It is not difficult to see that

$$\lim_{(t-t_0)\to\infty} \frac{d\bar{\rho}^*}{dt} = \begin{cases} 0 & (\alpha > 0), \\ \infty & (\alpha < 0). \end{cases}$$

This means that when energy is introduced the systems reach a stationary regime corresponding to an ideal gas, while when energy is removed all systems of the ensemble tend toward a limiting point of phase space, into which any selected flow of "probability fluid" flows. Systems which at the moment t_0

were infinitely far from the limiting point evolve toward it for an infinitely long time.

It is not difficult to consider the problem in a much more general case.

6. Equations for correlation functions. Acting in complete analogy with the method of paper ([2]), we obtain a chain of equations for the correlation functions $F_s(p_1, p_2, \dots, p_s, q_1, q_2, \dots, q_s)$

$$\frac{\partial F_s}{dt} = \{H_s; F_s\} - \sum_{1\le i\le s} \frac{\partial}{\partial p_i} \left(G(p_i, q_i, t) \cdot F_s\right) +$$

$$+v^{-1} \iint_\Omega \left\{ \sum_{1\le i\le s} \Phi\left(|q_i - q_{s+1}|\right); F_{s+1} \right\} dq_{s+1}\, dp_{s+1}.$$

Here Φ is the potential of the intermolecular forces, and the integration is performed over the 6-dimensional space.

The usual method of expansion in v^{-1} ([2]) leads to the system of equations

$$F_s = F_s^0 + v^{-1} F_s^{(1)} + v^{-2} F_s^{(2)} + \dots;$$

$$\frac{\partial F_s^0}{\partial t} = \{H_s; F_s^0\} - \sum_{1\le i\le s} \frac{\partial}{\partial p_i} (G_i, F_s^0);$$

$$\frac{\partial F_s^{(1)}}{\partial t} = \{H_s; F_s^{(1)}\} - \sum_{1\le i\le s} \frac{\partial}{\partial p_i} (G_i, F_s^{(1)}) + \int_\Omega \left\{ \sum_{1\le i\le s} \Phi(|q_i - q_{s+1}|); F_{s+1}^0 \right\} dp_{s+1}\, dq_{s+1}$$

and so on. The function H_s is the Hamiltonian function of a subsystem of s particles.

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REFERENCES

[1] S. Guiasu, *Lincei Rend. Sc. fis., mat. e nat.*, **39**, dicembre (1965).
[2] N. N. Bogolyubov, *Problems of Dynamical Theory in Statistical Physics*, 1957.

Note: Figure translations are in progress. See original paper for figures.