VARIATIONAL PRINCIPLES

MATHEMATICAL PHYSICS

1967

SovietRxiv

Abstract

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UDC 533.7

MATHEMATICAL PHYSICS

A. M. KOGAN

VARIATIONAL PRINCIPLES

FOR THE EQUATIONS OF THE KINETIC THEORY OF GASES

(Presented by Academician L. I. Sedov on 10 X 1966)

Recently notable progress has been achieved in the development of various models of continuous media and in the study of the general properties of these models. Variational principles play an important role in this general theory, making it possible to obtain equations for the description of models, and also to draw all those general conclusions that are usually obtained on the basis of the Lagrangian formalism.

A special feature of variational principles for the case of a continuous medium, in comparison, for example, with the case of a field, is the circumstance that one has to vary not only functions of spatial coordinates and time, but also particle trajectories, i.e., the particle coordinates as functions of time and of Lagrangian coordinates, assumed fixed. Another special feature is connected with the dissipative character of many equations of continuous media. Unlike conservative systems, a dissipative system cannot be characterized by a single density of the Lagrangian, and it is necessary additionally to introduce generalized dissipative forces. In this connection the variational principle is written as the equality to zero of the integral of a certain form linear in the variations, which does not reduce to the complete variation of some functional—the action of the system. All these questions are set forth in detail in ([1–3]).

Kinetic theory describes a gas in terms of distributions in the phase spaces of the canonical coordinates of the molecules. Thus in this theory a gas may be regarded as a kind of phase continuous medium. The purpose of the present note is to formulate variational principles for the Liouville equation, for the equations of the Bogolyubov chain, and for kinetic equations on the basis of the use of the concepts and methods characterized in ([1]).

1. Let a system of N particles have a Hamiltonian of the form

$$H = \sum_{\alpha=1}^{N} \frac{\mathbf{p}_\alpha^2}{2m} + \sum_{1\le\alpha<\beta\le N} \Phi(|\mathbf{q}_\alpha - \mathbf{q}_\beta|). \tag{1}$$

The distribution $f_N(t, \mathbf{q}_\alpha, \mathbf{p}_\alpha)$ in the N-particle phase Γ-space satisfies the Liouville equation

$$\partial f_N/\partial t = \{H; f_N\}, \tag{2}$$

for which we shall write a variational principle.

We write the phase trajectories in the form

$$q_\alpha^i = q_\alpha^i(t, \xi_\beta^j, \eta_\beta^j); \quad p_\alpha^i = p_\alpha^i(t, \xi_\beta^j, \eta_\beta^j), \quad (j, i = 1, 2, 3;\ \alpha, \beta = 1, 2, \dots, N), \tag{3}$$

where $\vec{\xi}_\beta, \vec{\eta}_\beta$ are the initial values of the canonical coordinates. The variations δq_α^i and δp_α^i are taken with $t, \vec{\xi}_\beta, \vec{\eta}_\beta$ fixed and, with the aid of (3), can be expressed in terms of $\mathbf{q}_\alpha, \mathbf{p}_\alpha$.

Taking into account the definition of f_N as the phase density, we shall regard the variational condition as satisfied

$$\delta(f_N dq_1 \dots dp_N) = 0. \tag{4}$$

We shall also use the equality

$$\frac{d}{dt}(f_N dq_1 \dots dp_N) = 0,$$

where d/dt is taken along any neighboring trajectory. Hence there follows the continuity equation

$$\frac{\partial f_N}{\partial t} + \sum_{\alpha=1}^{N} \left(\frac{\partial f_N \dot{q}_\alpha^i}{\partial q_\alpha^i} + \frac{\partial f_N \dot{p}_\alpha^i}{\partial p_\alpha^i} \right) = 0. \tag{5}$$

In what follows we shall choose δq_α^i and δp_α^i to be zero on the boundary of the region of integration. In this case, as is easy to see, (4) follows from (5).

To understand what the action for equation (2) looks like, let us write Hamilton' s principle for a system of N particles in the form

$$\delta S_\Gamma = \delta \int \left(\sum_{\alpha=1}^{N} \dot{q}_\alpha^i p_\alpha^i - H \right) dt = 0, \tag{6}$$

in which δq_α^i and δp_α^i are varied independently. In view of (4), one may, without violating (6), multiply S_Γ by $f_N dq_1 \dots dp_N$ and integrate over any region of the canonical variables. Thus the action for (1) has the form

$$S = \int_\Omega \left(\sum_{\alpha=1}^N \dot{q}_\alpha^i p_\alpha^i - H \right) f_N \, dt \, dq_1 \dots dp_N, \tag{7}$$

where Ω is any region of the space $(t, \mathbf{q}_1, \dots, \mathbf{p}_N)$.

Equating to zero the variation of the action (7), taken with account of (4), we obtain

$$\dot{q}_\alpha^i = \frac{\partial H}{\partial p_\alpha^i}; \qquad \frac{\partial p_\alpha^i f_N}{\partial t} + \sum_{\beta=1}^N \left(\frac{\partial \dot{q}_\beta^k p_\alpha^i f_N}{\partial q_\beta^k} + \frac{\partial \dot{p}_\beta^k p_\alpha^i f_N}{\partial p_\beta^k} \right) + f_N \frac{\partial H}{\partial q_\alpha^i} = 0. \tag{8}$$

The second equation (8), with the aid of (5), is reduced to the form

$$\dot{p}_\alpha^i = -\partial H / \partial q_\alpha^i.$$

Substituting now $\dot{q}_\alpha^i$ and $\dot{p}_\alpha^i$ into (5), we obtain equation (2).

2. The chain of Bogolyubov equations ([4]) has the form

$$\frac{\partial F_r}{\partial t} = \{H_r; F_r\} + \frac{1 - r/N}{v} \int \left\{ \sum_{\alpha=1}^r \Phi(|\mathbf{q}_\alpha - \mathbf{q}_{r+1}|); F_{r+1} \right\} dq_{r+1} dp_{r+1}. \tag{9}$$

In (9)

$$F_r = V^r \int f_N dq_{r+1} \dots dp_N; \qquad H_r = \sum_{\alpha=1}^r \frac{\mathbf{p}_\alpha^2}{2m} + \sum_{1 \le \alpha < \beta \le r} \Phi(|\mathbf{q}_\alpha - \mathbf{q}_\beta|);$$

$$v = \frac{V}{N}; \qquad V \text{ is the volume occupied by the gas.}$$

Equation (9) is an exact consequence of (2), but the function F_r contains less information than f_N. In accordance with this we shall consider a particular class of motions, which can be written in the form (3), where now $\alpha, \beta = 1, 2, \dots, r$. In addition, we shall assume $\delta q_\beta^i = \delta p_\beta^i = 0$ for $\beta > r$. In this case, from (4) and (5) there follow the equalities

$$\delta(F_r dq_1 \dots dp_r) = \delta(F_{r+1} dq_1 \dots dp_{r+1}) = 0, \tag{10}$$

and also

$$\frac{\partial F_r}{\partial t} + \sum_{\alpha=1}^{r} \left(\frac{\partial \dot{q}_\alpha^i F_r}{\partial q_\alpha^i} + \frac{\partial \dot{p}_\alpha^i F_r}{\partial p_\alpha^i} \right) = 0. \tag{11}$$

Taking into account that $\delta q_\beta^i = \delta p_\beta^i = 0$ for $\beta > r$, we obtain from (7)

$$S_r = V^r S \int \left(\sum_{\alpha=1}^{r} \dot{q}_\alpha^i p_\alpha^i - H_r \right) F_r \, dt \, dq_1 \dots dp_r -$$

$$- \frac{1 - r/N}{v} \int \sum_{\alpha=1}^{r} \Phi(|\mathbf{q}_\alpha - \mathbf{q}_{r+1}|) F_{r+1} \, dt \, dq_1 \dots dp_{r+1} + \text{const}. \tag{12}$$

Equating to zero δS_r, taken with account of (10), and using (11), we obtain

$$\dot{q}_\alpha^i = \frac{\partial H_r}{\partial p_\alpha^i}; \qquad F_r \dot{p}_\alpha^i + F_r \frac{\partial H_r}{\partial q_\alpha^i} + \frac{1 - r/N}{v} \left(\frac{\partial}{\partial q_\alpha^i} \sum_{\beta=1}^{r} \Phi(|\mathbf{q}_\alpha - \mathbf{q}_{r+1}|) F_{r+1} d\mathbf{q}_{r+1} d\mathbf{p}_{r+1} \right) = 0. \tag{13}$$

Equations (13) have the meaning of the equations of motion of a "liquid" phase particle. Differentiating the first equation (13) with respect to q_α^i and the second with respect to p_α^i, summing over i from 1 to 3 and over α from 1 to r, and substituting into the continuity equation (11), we obtain equation (9).

3. Let us consider the case $r = 1$, in which $N \to \infty$, $V \to \infty$, $v = \text{const}$,

$$\frac{\partial F_1}{\partial t} = \{H_1; F_1\} + \frac{1}{v} \int \{\Phi(|\mathbf{q}_1 - \mathbf{q}_2|); F_2\} \, d\mathbf{q}_2 d\mathbf{p}_2. \tag{14}$$

In (4) it is shown that, for a rarefied gas under the assumption of a small change of F_1 at distances of the order of the molecular dimensions,

$$F_2(t, \mathbf{q}_1, \mathbf{p}_1, \mathbf{q}_2, \mathbf{p}_2) = F_1(t, \mathbf{q}_1, \mathbf{P}_1) \, F_1(t, \mathbf{q}_1, \mathbf{P}_2). \tag{15}$$

In (15), $\mathbf{P}_1$ and $\mathbf{P}_2$ denote the momenta that the molecules must have at $t = -\infty$ so that, in the auxiliary two-body problem with scattering potential Φ, at $t = 0$ they acquire the values of the canonical coordinates equal to $\mathbf{q}_1, \mathbf{p}_1$ and $\mathbf{q}_2, \mathbf{p}_2$, respectively. Taking (15) into account, we write (14) in the form

$$\frac{\partial F_1}{\partial t} = \{H_1; F_1\} + \frac{1}{v} \int \{\Phi(|\mathbf{q}_1 - \mathbf{q}_2|); F_1(t, \mathbf{q}_1, \mathbf{P}_1) F_1(t, \mathbf{q}_2, \mathbf{P}_2)\} \, d\mathbf{q}_2 d\mathbf{p}_2. \tag{16}$$

In (4) it is noted that (16) is only another form of writing the classical Boltzmann equation (for a detailed proof see (5)).

According to (12),

$$S_1 = \int (\dot{q}_1^i p_1^i - H_1) F_1 \, dt \, d\mathbf{q}_1 d\mathbf{p}_2 - \frac{1}{v} \int \Phi(|\mathbf{q}_1 - \mathbf{q}_2|) F_2 \, dt \, d\mathbf{q}_1 d\mathbf{p}_1 d\mathbf{q}_2 d\mathbf{p}_2. \quad (17)$$

Equation (11) takes the form

$$\partial F_1/\partial t + \partial \dot{q}_1^i F_1/\partial q_1^i + \partial \dot{p}_1^i F_1/\partial p_1^i = 0. \quad (18)$$

Substitution of F_2 from (15) into (17) makes S_1 depend only on F_1. If we now vary S_1, it is not possible to satisfy the necessary second condition (10), taken at $r = 1$. Therefore we first take the variation of (17) under the conditions (10) with $r = 1$ and only then use (15). This gives

$$\delta \int (\dot{q}_1^i p_1^i - H_1) F_1 \, dt \, d\mathbf{q}_1 d\mathbf{p}_1 + \int Q_i \, \delta q_1^i \, dt \, d\mathbf{q}_1 d\mathbf{p}_1 = 0, \quad (19)$$

where

$$Q_i = -\frac{1}{v} \int \frac{\partial \Phi(|\mathbf{q}_1 - \mathbf{q}_2|)}{\partial q_1^i} F_1(t, \mathbf{q}_1, \mathbf{P}_1) F_1(t, \mathbf{q}_1, \mathbf{P}_2) \, d\mathbf{q}_2 d\mathbf{p}_2. \quad (20)$$

From (19) and (20), taking into account the first condition (10) for $r = 1$ and (18), we obtain

$$\dot{q}_1^i = \frac{\partial H_1}{\partial p_1^i}; \qquad F_1 \dot{p}_1^i + F_1 \frac{\partial H_1}{\partial q_1^i} + \frac{1}{v} \int \frac{\partial \Phi}{\partial q_1^i} F_1(t, \mathbf{q}_1, \mathbf{P}_1) F_1(t, \mathbf{q}_1, \mathbf{P}_2) \, d\mathbf{q}_2 d\mathbf{p}_2 = 0. \quad (21)$$

Differentiating the first equation (21) with respect to q_1^i, and the second with respect to p_1^i and substituting into (18), we obtain (16).

The derivation of the Boltzmann equation from the variational principle (19), (20) with the additional condition (18) appears instructive for the following reasons.

First, the dissipativity introduced by equality (15) has "destroyed" the action (17) and automatically led us to the form (19), which is postulated in ([1]) for dissipative systems. In this way a natural expression (20) has been obtained for the density of the generalized force.

Second, the very writing of Q_i in the form of a sixfold integral predetermines the inevitability of obtaining the Boltzmann equation not in its classical form, but in the form (16).

Third, the very possibility of writing the Boltzmann equation in the form of the continuity equation (18) and of the equations of motion of a "fluid" phase particle (21) appears to be of interest.

Let us note that (19) also serves as a variational principle for the Bogolyubov equation ([4]), which takes into account the change of F_1 over lengths of the order of molecular dimensions. The matter reduces to a small change of Q_i from (20). It is just as easy to see that, in order to obtain a variational principle for the case of dense gases, one must write $\delta S_2 = 0$ taking (10) into account, and then in the resulting expression use one or another superposition approximation.

The author expresses his gratitude to L. I. Sedov for posing the problem and for discussions.

Institute of Chemical Physics
Academy of Sciences of the USSR

Received
20 IX 1966

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