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ON A VARIATIONAL PRINCIPLE OF STATISTICAL MECHANICS

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The variational principle for the Hamilton-Jacobi equation is formulated and proved. The variational principle is stated in terms of Gibbs ensemble from statistical mechanics. The varied functional is the expectation of the functional of action of analytical mechanics; the Hamilton-Jacobi equation is represented by an Euler equation in case of variation of the distribution function.

The close relationship between first-order partial derivative equations and ordinary differential equations is well known. In analytical mechanics, its counterpart is the relationship between the Hamilton-Jacobi equation and the Hamilton equations. Since Hamilton equations can be obtained from the variational principle, it can be expected that a certain variational principle exists also for the Hamilton-Jacobi equation. That variational principle cannot be of the same type as the ordinary integral variational principles because Euler's equations for them are partial derivative equations of at least second order, while the Hamilton-Jacobi equation is a first-order equation. In this paper we offer a statement and a proof of the variational principle for the Hamilton-Jacobi equation. We will show that a natural construction in terms of which the variational principle can be formulated is the Gibbs ensemble of statistical mechanics; the varied functional is the expectation of the action of analytical mechanics, while the Hamilton-Jacobi equation is an Euler equation when the distribution function is varied. This statement can be viewed also as the initial postulate of statistical mechanics.

Consider a mechanical system with generalized coordinates \(q_1, q_2, \ldots, q_n\), momenta \(p_1, \ldots, p_n\), and the Hamiltonian \(H(p, q, t)\) (the letters \(p, q\) symbolize the set of coordinates \(p_1, \ldots, p_n\), \(q_1 \ldots, q_n\)). Take a Gibbs ensemble of such systems with the distribution function density \(f(p, q, t)\). In the Gibbs ensemble the velocities of the motion \(p, q\) of the points representing the system state in the space \(R\) of the variables \(p, q\) can be viewed as functions of \(p, q, t\). The function \(f(p, q, t)\) then satisfies the continuity equation

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\[
\frac{\partial f}{\partial t} + \frac{\partial (\dot{q}_i f)}{\partial q_i} + \frac{\partial (\dot{p}_i f)}{\partial p_i} = 0.
\] (1)

The superscripts run the values 1, ..., n; summation is taken over like superscripts.

Introduce certain "Lagrangian coordinates" of the system's paths – the functions \(n_a(p, q, t) (a=1, ..., n)\), which remain invariable along the paths:

\[
\frac{\partial n_a}{\partial t} + \dot{q}_i \frac{\partial n_a}{\partial q_i} + \dot{p}_i \frac{\partial n_a}{\partial p_i} = 0.
\] (2)

Consider the functional

\[
I = \int_{t_0}^{t_1} \left[ \int_R \left[ \left[ \frac{\partial f}{\partial \dot{q}_i} - \frac{\partial n_a}{\partial q_i} \dot{q}_i + \frac{\partial n_a}{\partial p_i} \dot{p}_i \right] \right] dpdqdt - \int_R \psi(q, \pi) f(p, q, t) dpdq.
\] (3)

Here the function \(\psi(q, \pi)\) is considered to be the given function of the arguments \(\dot{q}_i\) and \(n_a\) and the function \(f(p, q, t)\) for each \(t\) is assumed to be decreasing at infinity with a rate sufficient for convergence of the integrals.

The first term in (3) has the sense of the expectation of the functional of action of analytical mechanics; the second term, as will be seen from the subsequent discussion, is connected with the flow of momentum at \(t = t_1\).

Consider the stationary points of the functional (3) on a set of the functions \(f(p, q, t), \dot{q}_i(p, q, t), \dot{p}_i(p, q, t)\) and \(n_a(p, q, t)\), subject to constraints (1), (2), and the initial conditions

\[
f = \psi(q, \pi) \left| \frac{\partial n_a}{\partial p_i} \right| \text{ for } t = t_0,
\] (4)

where \(\psi(q, \pi)\) is a given function and \(|\partial n_a/\partial p_i|\) is the determinant of the matrix \(|\partial n_a/\partial p_i|\).

Variational principle. At the stationary points of functional (3), the functions \(\dot{q}_i, \dot{p}_i\) satisfy Hamilton equations; the Lagrange multiplier for constraint (1) satisfies the Hamilton-Jacobi equation.

We propose to demonstrate the above assertion. Write Euler equations of functional (3). Denote by \(\alpha\) and \(\theta_{\alpha}^f\) the Lagrange multipliers for constraints (1), (2). Euler equations are then found by varying the functional

\[
\int_{t_0}^{t_1} \left[ \int_R \left[ \left[ \left[ \frac{\partial f}{\partial \dot{q}_i} - \frac{\partial n_a}{\partial q_i} \dot{q}_i + \frac{\partial n_a}{\partial p_i} \dot{p}_i \right] \right] \right] dpdqdt - \int_R \psi(q, \pi) f(p, q, t) dpdq.
\]

It we obtain the following equations: by varying in \(\dot{q}_i(p, q, t)\) —

\[
\frac{\partial n_a}{\partial q_i} - \theta_{\alpha}^f \frac{\partial n_a}{\partial q_i} = p_i;
\] (5)

by varying in \(\dot{p}_i(p, q, t)\) —
by varying in
\[
\frac{\partial \alpha}{\partial \rho_i} + \theta_a \frac{\partial \pi_a}{\partial \rho_i} = 0;
\] (6)

by varying in
\[
\rho_i \dot{\alpha} - H - \frac{\partial \alpha}{\partial t} \dot{q}_i - \frac{\partial \alpha}{\partial q_i} \dot{\alpha} - \rho_i \frac{\partial \alpha}{\partial \rho_i} - \theta_a \left( \frac{\partial \pi_a}{\partial t} + \dot{q}_i - \frac{\partial \pi_a}{\partial q_i} + \dot{\alpha} \frac{\partial \pi_a}{\partial \alpha} \right) = 0;
\] (7)

by varying in
\[
\frac{\partial (\theta_a f)}{\partial t} + \frac{\partial (\theta_a f)}{\partial q_i} + \frac{\partial (\theta_a f)}{\partial \rho_i} = 0.
\] (8)

A variation in \( \alpha \) and \( \theta_a \) leads to equations of relationships (1) and (2). In writing the equations we assume that a region of space \( R \) is considered in which \( f > 0 \).

By virtue of the arbitrariness of the variations \( \delta f \) and \( \delta \pi_a \) at \( t = t_1 \), the following relations follow from the stationarity of the functional
\[
\alpha = \varphi(q, \pi) \text{ at } t = t_1, \quad (9)
\]
\[
\theta_a = \frac{\partial \varphi}{\partial \pi} = 0 \text{ at } t = t_1. \quad (10)
\]

We have now only to write the condition following from the equality
\[
\int_R (\alpha \delta f + \theta_a [\delta \pi_a]) |_{t=t_1} d\rho dq = 0. \quad (11)
\]

It will be shown below that equality (11) is fulfilled automatically by virtue of Eqs. (4) and (6).

We now proceed to the analysis of Eqs. (5)-(10). Equation (7) can be rewritten by using (5) and (6) in a simpler form:
\[
\frac{\partial \alpha}{\partial t} - \frac{\partial \alpha}{\partial q_i} \dot{q}_i + H(p, q, t) = 0.
\] (12)

Suppose that functions \( \pi(p, q, t) \) at each \( q, t \) determine a one-to-one mapping \( p \leftrightarrow \pi \) so that \( p \) can be considered the functions of \( t, q, \pi : p = p(\pi, q, t) \) and
\[
|\partial \pi/\partial p| \neq 0. \quad (13)
\]

Then all the functions of \( p, q, \) and \( t \) can also be considered to be functions of \( \pi, q, t \). In particular, \( \alpha = \alpha(\pi, q, t) \). Equations (5) and (6) in terms of the functions \( \alpha(\pi, q, t) \) assume a simple form (taking into account (13)):
\[
\frac{\partial \alpha}{\partial t} = \rho_i, \quad (14)
\]
\[
\frac{\partial \alpha}{\partial \alpha} = \theta_a. \quad (15)
\]

By \( \partial_1 \alpha \) and \( \partial_2 \alpha \) we denoted the derivatives of \( \alpha \) with respect to \( q_1 \) and \( \pi_a \), respectively, at constant \( \pi, t \) and \( q, t \). Equations (14), (15) define a canonical transformation of \( p, q \rightarrow \pi, \theta \) (see [1, §9.1]).

By virtue of (14) and (15), (12) can be rewritten as a Hamilton-Jacobi equation for the function \( \alpha(\pi, q, t) \):

10
\[ \partial_t \alpha + H(\partial_t \alpha, q, t) = 0. \]  

(16)

Here \( \partial_t \alpha \) is a derivative of \( \alpha \) with respect to \( t \) at constant \( \pi, q \).

Equation (16), together with condition (9), constitutes the Cauchy problem for the function \( \alpha \).

Note that assumption (13) is satisfied a priori if the determinant of the matrix \( \| \partial^2 q / \partial q_i \partial q_n \| \) is nonzero and \( t_1 - t_0 \) is sufficiently small. Indeed, for small \( t_1 - t_0 \) and smooth \( \phi \) and \( H \), we can guarantee the unique existence of a smooth solution to Cauchy problem (16), (9) (see [2, \$47]). By virtue of (14), the determinant of the matrix \( \| \partial p_i / \partial q_n \| \) coincides with the determinant of the matrix \( \| \partial^2 q / \partial q_i \partial q_n \| \); by virtue of (9) at \( t = t_1 \), it coincides with the determinant of the matrix \( \| \partial^2 q / \partial q_i \partial q_n \| \). By continuity, it will be nonzero over a sufficiently small time interval.

We will show that at a stationary point, the following Hamilton equations hold:

\[ \dot{p}_i = -\frac{\partial H}{\partial q_i}, \quad \dot{q}_i = \frac{\partial H}{\partial p_i}. \]  

(17)

Auxiliary equations will be needed:

\[ \frac{\partial q}{\partial p} \frac{\partial q}{\partial q} \frac{\partial q}{\partial q} \frac{\partial q}{\partial q} = 0, \quad \frac{\partial q}{\partial q} \frac{\partial q}{\partial q} \frac{\partial q}{\partial q} \frac{\partial q}{\partial q} = 0, \]  

(18)

These equations can be proved by differentiating (5) and (6) with respect to \( p_i, q_i \):

\[ \frac{\partial q}{\partial q} \frac{\partial q}{\partial q} \frac{\partial q}{\partial q} \frac{\partial q}{\partial q} = 0, \]  

(19)

Alternating in \( i, j \) the first and the last equality and subtracting from the second equality the third equality, we obtain relations (18).

Let us differentiate (12) with respect to \( p \) and \( q \). Making use of (6) and (7) we have

\[ \frac{\partial q}{\partial q} \frac{\partial q}{\partial q} \frac{\partial q}{\partial q} \frac{\partial q}{\partial q} = \frac{\partial H}{\partial q}, \]  

(20)

\[ \frac{\partial q}{\partial q} \frac{\partial q}{\partial q} \frac{\partial q}{\partial q} \frac{\partial q}{\partial q} = \frac{\partial H}{\partial q}. \]  

(21)
Substituting here the expression for $\partial \pi_\alpha / \partial t$ in terms of $\dot{p}$, $\dot{q}$ from (2) and the corresponding expression for $\partial \theta_\alpha / \partial t$ from the equation

$$\frac{\partial \theta_\alpha}{\partial t} + \dot{q}_i \frac{\partial \theta_\alpha}{\partial q_i} + \dot{p}_i \frac{\partial \theta_\alpha}{\partial p_i} = 0,$$

which follows from (8) and (1), and making use of relation (18), we obtain the Hamilton equations (17).

Equation (1), by virtue of Hamilton equation (17), is transformed into the Liouville equation

$$\frac{\partial f}{\partial t} + \frac{\partial H}{\partial p_i} \frac{\partial f}{\partial q_i} - \frac{\partial H}{\partial q_i} \frac{\partial f}{\partial p_i} = 0.$$

This system of equations is solved as follows. First we solve the Cauchy problem (16), (9). From its solution $a(p, q, t)$, we find from Eq. (14) the functions $\pi_\alpha(p, q, t)$. The values of these functions are substituted into the initial data (4), and the initial value $f(p, q, t_0)$ of the function $f$ is found. The Cauchy problem is then solved for Liouville equation (1), (16). The functions $\theta_\alpha$ are reconstructed from $a(p, q, t)$ using Eq. (15). If $\varphi = q_\alpha \pi_\alpha$, then "the Lagrangian coordinates" $\pi_\alpha$, by virtue of (14) have the sense of momenta at the final time point $t = t_1$, and $\psi(q, \pi)$ have the sense of the density of the simultaneous distribution of the initial coordinate value and the final momentum value.

Equation (10) is satisfied as an identity by virtue of (15) and (9). We will show that Eq. (11) is also satisfied as an identity.

Calculate the variation of the function $f$ at $t = t_0$. To this end we need the equality

$$\delta \left| \frac{\partial \pi}{\partial p} \right| = \left| \frac{\partial \pi}{\partial p} \right| \frac{\partial \delta \pi_\alpha}{\partial \pi_\alpha}. \quad (19)$$

Its validity can be verified as follows:

$$\delta \left| \frac{\partial \pi}{\partial p} \right| = \left( \frac{\partial}{\partial (\partial \pi_\alpha/\partial p_i)} \left| \frac{\partial \pi}{\partial p} \right| \right) \frac{\partial \delta \pi_\alpha}{\partial p_i} = \left| \frac{\partial \pi}{\partial p} \right| \frac{\partial \pi_\alpha}{\partial p_i} \frac{\partial \delta \pi_\alpha}{\partial p_i} = \left| \frac{\partial \pi}{\partial p} \right| \frac{\partial \delta \pi_\alpha}{\partial \pi_\alpha}.$$

We have used here a formula for the components of the inverse matrix

$$\frac{\partial}{\partial (\partial \pi_\alpha/\partial p_i)} \left| \frac{\partial \pi}{\partial p} \right| = \left| \frac{\partial \pi}{\partial p} \right| \frac{\partial \pi_\alpha}{\partial p_i}.$$

According to the initial condition (4) and formula (19), we have for the variation of the function $f$,

$$\delta f = \frac{\partial \varphi}{\partial \pi_\alpha} \delta \pi_\alpha \left| \frac{\partial \pi}{\partial p} \right| + \psi \left| \frac{\partial \pi}{\partial p} \right| \frac{\partial \delta \pi_\alpha}{\partial \pi_\alpha} = \left| \frac{\partial \pi}{\partial p} \right| \frac{\partial (\psi \delta \pi_\alpha)}{\partial \pi_\alpha}.$$

Therefore
\[
\int \alpha \delta f dp dq = \int \alpha \left[ \frac{\partial \pi}{\partial p} \frac{\partial (\alpha \psi_{\alpha})}{\partial \pi_{\alpha}} \right] dp dq = \\
= \int \alpha \frac{\partial (\psi_{\alpha})}{\partial \pi_{\alpha}} dp dq = \int \psi_{\alpha} \alpha \pi_{\alpha} dp dq = \int \psi_{\alpha} \alpha \pi_{\alpha} dp dq.
\]

(20)

From equality (20) it follows that relation (11) is satisfied as an identity by virtue of (15). This completes the proof of the variational principle stated above.

It should be noted that constraint (2) could be replaced by the constraint

\[
\frac{\partial (n_{\alpha})}{\partial \pi} + \frac{\partial (n_{\alpha} \dot{v})}{\partial \dot{v}} + \frac{\partial (n_{\alpha} \ddot{v})}{\partial \ddot{v}} = 0,
\]

in which case the Lagrange multiplier for constraint (1) would have the sense of Legendre transform of the function \(\alpha(\pi, q, t)\) in variables \(\pi_{\alpha}\), and would be a function of \(\theta, q, t\).

The variational principle for functional (3) is close philosophically to the Morse-Feschbach principle (see [3, §11, chapter III]), where the value of one of the sought-for functions is given at \(t = t_0\) and the value of the other function at \(t = t_1\) (in contrast to the Morse-Feschbach principle, the Hamilton-Jacobi equations and the Liouville equation are not conjugated in the ordinary sense). Another close analogue is the variational principle for an ideal compressible liquid flow in Euler coordinates (see [3, §5, chapter III]).

If for the function \(\psi(q, \pi)\) we take \(\delta\)-function, then the statement formulated in the paper becomes the Hamilton principle for a mechanical system with given coordinates \(q\) at \(t = t_0\). The values of momentum at \(t = t_1\) are obtained as a natural boundary condition. We can indicate a modification of the variational principle that is tantamount to specifying the positions of the particles at \(t = t_0\) and \(t = t_1\). Instead of \(n\) "Lagrangian coordinates" \(\pi_{\alpha}\), in that case, \(2n\) coordinates are introduced, half of which takes the given values at \(t = t_0\) and the other half at \(t = t_1\).

The statement proved in this paper has been first announced in publication [4].

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