PHYSICS

1961

SovietRxiv

Abstract

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PHYSICS

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THE VIRIAL THEOREM FOR THE CLASSICAL PROBLEM OF SCATTERING OF PARTICLES BY A FORCE CENTER

(Presented by Academician V. A. Fock on 26 XII 1960)

The virial theorem was first proved in classical mechanics for finite motions—those for which the coordinates and momenta of the material points making up the system are bounded. In quantum mechanics the theorem was proved already in (1,2) for stationary states of the discrete spectrum, i.e., for bound states, which corresponds to the condition of finiteness in classical mechanics.

V. A. Fock showed (3) that the most natural derivation of the virial theorem is the use of the variational principle and of a variation of the length scale. The corresponding formulas were derived for classical mechanics (4), for the Schrödinger equation (3), the Dirac equation (3), in the Thomas-Fermi method (5), etc. However, all these proofs referred to bound states or to finite motions. For problems of the continuous spectrum of the energy operator in quantum mechanics, a formula analogous to the virial theorem was first obtained by the author (6) for the problem of scattering of particles by a force center. Subsequently this formula was generalized to more complicated problems of collision theory—inelastic, exchange processes, etc. (7,8), to the Dirac equation and to problems of quantum field theory (9). Meanwhile, in classical mechanics the corresponding generalization has not yet been carried out.

Let us show, by a concrete example, how to obtain this generalization. First we shall find a general formula from which the virial theorem can be obtained for any classical problem. We start from Hamilton' s variational principle. Let

$$S = \int_{t_1}^{t_2} L(q_1, \dots, q_n;\ \dot{q}_1, \dots, \dot{q}_n;\ t)\, dt \tag{1}$$

be the action functional, depending on the generalized coordinates $q_i(t)$, $i = 1, 2, \dots, n$. Then, assuming that $q_i(t)$ correspond to the real motion, we have for the variation δS the formula

$$\delta S = \sum_{i=1}^{n} \frac{\partial L}{\partial \dot{q}_i}\, \delta q_i \Bigg|_{t_1}^{t_2}, \tag{2}$$

where we assume that the variations $\delta q_i(t)$ do not necessarily vanish at the ends of the time interval.

Now consider the special case of variations

$$\delta q_i(t) = \varepsilon q_i(t), \tag{3}$$

where ε is an infinitesimal parameter. We shall call such a transformation a variation of scale. Substituting (3) into formulas (1) and (2) and neglecting quantities proportional to ε^2, we obtain

$$\int_{t_1}^{t_2} \sum_{i=1}^{n} \left(\frac{\partial L}{\partial \dot{q}_i} \dot{q}_i + \frac{\partial L}{\partial q_i} q_i \right) dt = \sum_{i=1}^{n} \frac{\partial L}{\partial \dot{q}_i} q_i \Bigg|_{t_1}^{t_2}. \tag{4}$$

Applying formula (4) to various systems and to various types of motion, we can obtain the virial theorem for each particular case. For example, averaging the right- and left-hand sides of the formula over a long time interval for finite motions, or over a period for periodic motions, we obtain zero on the right-hand side and arrive at the usual formulation of the theorem. We note, moreover, that both the left- and right-hand sides of equality (4) depend essentially on the choice of generalized coordinates. By choosing different generalized coordinates, we shall, generally speaking, obtain different formulations.

For infinite motions, when $t_1 \to -\infty$ or $t_2 \to +\infty$, both sides of formula (4) increase without bound, and this complicates the proof.

Let us consider the problem of scattering of a particle of mass $m = 1$ by a spherically symmetric force center. In this case the Lagrange function has the form

$$L = \frac{v^2}{2} - U(r). \tag{5}$$

Choosing the Cartesian coordinates x, y, z as generalized coordinates, we obtain from formula (4)

$$\int_{t_1}^{t_2} \left(v^2 - r\frac{dU}{dr} \right) dt = \mathbf{v} \cdot \mathbf{r} \Big|_{t_1}^{t_2}. \tag{6}$$

Let, as $|t| \to \infty$, the particle move with velocity v_∞. Suppose further that the instant $t = 0$ corresponds to the minimum value $r = r_0$. Then the motion is symmetric with respect to the vector $\mathbf{r}_0 = \mathbf{r}(0)$, and for large $|t|$ we have

$$r = s + v_\infty |t|. \tag{7}$$

It follows that both sides of formula (6), as $t_1 \to -\infty$, $t_2 \to +\infty$, contain the increasing term $v_\infty^2(t_2 - t_1)$. Subtracting this term and taking into account the law of conservation of energy

$$\frac{v^2}{2} + U = \frac{v_\infty^2}{2}, \tag{8}$$

we have

$$\int_{t_1}^{t_2} \left(2U + r\frac{dU}{dr}\right) dt = (v_\infty^2 t - \mathbf{v}\cdot\mathbf{r})\Big|_{t_1}^{t_2}. \tag{9}$$

Now we can pass to the limit $t_1 \to -\infty,\ t_2 \to \infty$. We obtain

$$\int_0^\infty \left(2U + r\frac{dU}{dr}\right) dt = v_\infty \lim_{t\to\infty} (v_\infty t - r) = -\, v_\infty s. \tag{10}$$

Here we have taken into account the symmetry of the motion, as well as the fact that $\mathbf{r}_0 \cdot \mathbf{v}_0 = 0$.

Thus, on the left-hand side of formula (10) stands an expression characteristic of the virial theorem, while on the right-hand side is the quantity s, which has a simple geometric meaning: it is equal to the distance by which, as $t \to \infty$, the particle has advanced in comparison with a point which begins at $t = 0$ from the origin and moves uniformly with speed v_∞ along a straight line, catching up with the scattered particle. However, the right-hand side of equation (10) can also be given another meaning, making it possible to compare it with the corresponding quantum-mechanical expression. For this purpose we shall represent it in the form of an integral.

in terms of r. We denote the angular momentum of the particle by

$$M = r^2\dot{\varphi} = \rho v_\infty, \tag{11}$$

where ρ is the impact parameter. Using formula (8), we obtain

$$t(r) = \int_{r_0}^{r} \frac{dr}{\sqrt{v_\infty^2 - 2U - M^2/r^2}} = \int_{r_0}^{r} \frac{dr}{v_r}, \tag{12}$$

where $r = r_0$ is the value at which $v_r = \dot{r}(r)$ vanishes. Hence we obtain

$$\lim_{t\to\infty} [v_\infty t - r(t)] = \lim_{r\to\infty} [v_\infty t(r) - r] = \lim_{r\to\infty} \left(\int_{r_0}^{r} \frac{v_\infty}{v_r}\, dr - r \right). \tag{13}$$

Let us now consider the expression for the phase of the wave function in the semiclassical method (see, for example, [10], § 111)

$$\eta(v_\infty, M) = \lim_{r\to\infty} \left[\int_{r_0}^{r} \sqrt{v_\infty^2 - 2U - M^2/r^2}\, dr - \int_{\rho}^{r} \sqrt{v_\infty^2 - M^2/r^2}\, dr \right]. \tag{14}$$

The second integral can readily be evaluated for large r. We obtain

$$\eta(v_\infty, M) = \lim_{r\to\infty} \left(\int_{r_0}^{r} v_r\, dr - v_\infty r + M\frac{\pi}{2} \right). \tag{15}$$

Comparing this expression with formula (13), it is easy to see that

$$\lim_{t\to\infty} [v_\infty t - r] = -\frac{\partial \eta}{\partial v_\infty}. \tag{16}$$

We note that, although r_0 and ρ depend on v_∞, this dependence need not be taken into account in differentiating, since in formula (15) the function v_r under the integral sign vanishes at the lower limit. Thus, finally, we obtain

$$\int_0^\infty \left(2U + r\frac{dU}{dr} \right) dt = v_\infty \frac{\partial \eta}{\partial v_\infty}. \tag{17}$$

This formula may be compared with the corresponding equality in quantum mechanics [6–8]

$$2\int_0^\infty \left(2U + r\frac{dU}{dr} \right) \psi_l^2(r)\, dr = v_\infty^2 \frac{d\eta_l}{dv_\infty}, \tag{18}$$

where ψ_l is the radial function of the l-th partial wave, having the asymptotic form

$$\psi_l \sim \sin\left(kr - \frac{l\pi}{2} + \eta_l \right), \tag{19}$$

and η_l is the phase of this radial function. We have here set Planck' s constant $\hbar$ equal to unity; then the azimuthal quantum number l coincides, for large l, with M.

The transition from the quantum formula (18) to the classical formula (17) can be traced if, in formula (18), one substitutes for $\psi_l(r)$ the semiclassical function

$$\psi_M(r) = \sqrt{\frac{v_\infty}{v_r}} \sin\left(\int_{r_0}^{r} v_r\, dr + \frac{\pi}{4}\right), \tag{20}$$

phase of which coincides with the phase in formula (15). Assuming now that for $r < r_0$ the function decreases so rapidly that it may be set equal to zero, and for $r > r_0$ oscillates so rapidly that one may set

$$\psi_M^2 = \frac{1}{2}\frac{v_\infty}{v_r}, \tag{21}$$

we arrive at the desired relation between the two formulas.

For stationary bound states with energy E and with radial wave function ψ_E, we have the analogous formula

$$\int_0^\infty \left(2U + r\frac{dU}{dr}\right)\psi_E^2\, dr = 2E, \tag{22}$$

and, finally, for finite motions in classical mechanics,

$$\int_{t_1}^{t_2} \left(2U - 2E + r\frac{dU}{dr}\right) dt = 0, \tag{23}$$

where the integration may be carried out, for example, between two instants of time when $\mathbf{r}$ and $\mathbf{v}$ are orthogonal (the instants of greatest and least distance of the point from the force center).

Let us note in conclusion that the angle of deflection of the particle in scattering θ and the differential effective cross section σ are also simply expressed through derivatives of the semiclassical phase (11)

$$\theta = 2\frac{\partial\eta}{\partial M}; \qquad \sigma = -\frac{M}{2v_\infty^2}\left(\frac{\partial^2\eta}{\partial M^2}\right)^{-1}. \tag{24}$$

For more complicated problems, for example for a system of interacting particles, the proof of the theorem becomes more complicated, since as $|t| \to \infty$ the Lagrange function, generally speaking, does not tend to a constant value. In this case one must consider the difference between the complete Lagrange function

L and the limiting L_-—as $t \to -\infty$, or L_+—as $t \to \infty$, in which the interaction of systems of particles moving apart from one another is not taken into account.

It is curious to note that in quantum mechanics this theorem was proved earlier than in classical mechanics—a case apparently exceptional.

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Received
8 XII 1960

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