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TRANSFORMATION GROUPS AND THE VIRIAL THEOREM

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A generalization of Noether's result for classical mechanics is given, which shows that the virial theorem is related to an invariance property of the Lagrange function. Two examples are discussed in detail.

1. In classical mechanics integrals of the motion play an essential role; accordingly their theory has been elaborated in great detail and generality, culminating in Noether's fundamental theorem, which connects them with continuous invariance groups of the action integral. The virial theorem, however, in spite of its physical significance, has a somewhat separate position and is hardly connected with the main theory. It is the purpose of this note to remedy this situation by showing that virial theorems can be derived by means of a generalization of Noether's idea.

2. Let q_k $(k=1, 2, \ldots, n)$ be a set of n functions of t, obeying n differential equations of motion derivable from a Lagrange function $L(t, q, \dot{q})$,

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_k}-\frac{\partial L}{\partial q_k}=0. \tag{1}$$

Note that the equations are not affected if one adds to L the total time derivative of an arbitrary function $\Omega(t, q)$, or if one multiplies L by an arbitrary constant $a\neq 0$.

3. Consider an infinitesimal coordinate transformation in the $(n+1)$-dimensional (t, q)-space

$$t'=t+\varepsilon\varphi(t, q), \qquad q'_k=q_k+\varepsilon\chi_k(t, q).$$

(Observe that φ is allowed to depend on q_k, which is somewhat more general than in most treatments.) The transformed derivatives are

$$\frac{dq'_k}{dt'}\equiv\dot{q}'_k=\dot{q}_k+\varepsilon\left(\frac{d\chi_k}{dt}-\dot{q}_k\frac{d\varphi}{dt}\right),$$

where d/dt denotes again total differentiation.

Choose n functions $q_k(t)$ so as to define a curve in (t, q)-space. For any finite arc of that curve the action integral can be expressed in either set of coordinates,

$$\int L(t, q, \dot{q})\, dt = \int L'(t', q', \dot{q}')\, dt'. \tag{2}$$

The relation between the differentials is

$$dt' = \left(1 + \varepsilon \frac{d\varphi}{dt}\right) dt,$$

because the integral is taken along the curve. For prescribed L equation (2) defines the transformed Lagrange function L' up to a total derivative,

$$L'(t', q', \dot{q}')\left(1 + \varepsilon \frac{d\varphi}{dt}\right) = L(t, q, \dot{q}) + \varepsilon \frac{d\Omega(t, q)}{dt}.$$

4. The action integral is *invariant* when the function L' is the same as L, apart from a total derivative,

$$L(t', q', \dot{q}')\left(1 + \varepsilon \frac{d\varphi}{dt}\right) = L + \varepsilon \frac{d\Omega}{dt}. \tag{3}$$

Collecting the terms of first order in ε one finds for this invariance condition

$$\frac{\partial L}{\partial t}\varphi + \frac{\partial L}{\partial q_k}\chi_k + \frac{\partial L}{\partial \dot{q}_k}\left(\frac{d\chi_k}{dt} - \dot{q}_k \frac{d\varphi}{dt}\right) + L\frac{d\varphi}{dt} = \frac{d\Omega}{dt}.$$

This should hold for all functions $q_k(t)$; for those that obey the equations of motion (1) the left-hand side can be transformed by some algebra into

$$\frac{d}{dt}\left[\frac{\partial L}{\partial \dot{q}_k}(\chi_k - \dot{q}_k \varphi) + L\varphi\right] = \frac{d\Omega}{dt}. \tag{4}$$

Hence one finds that

$$\Psi(t, q, \dot{q}) = \frac{\partial L}{\partial \dot{q}_k}(\chi_k - \dot{q}_k \varphi) + L\varphi - \Omega$$

is a constant of the motion—which is Noether's theorem for classical mechanics.

5. The invariance condition (3) implies that the equations of motion themselves are also invariant; i.e., when expressed in the variables t', q_k' they have the same form as in t, q_k. On the other hand, (3) is not necessary for invariance of the equations of motion: for instance the weaker condition

$$L(t', q', \dot{q}')\left(1 + \varepsilon \frac{d\varphi}{dt}\right) = aL + \varepsilon \frac{d\Omega}{dt}, \tag{5}$$

with constant $a = 1 + \varepsilon\alpha$, is already sufficient. We shall show that *this weaker invariance condition leads to a virial theorem.*

The same algebra as used in 4 now leads to an additional term in (4)

$$\frac{d}{dt}\left[\frac{\partial L}{\partial \dot{q}_k}(\chi_k - \dot{q}_k\,\varphi) + L\varphi - \Omega\right] = \alpha L\,.$$

Integrating from t_1 to t_2, dividing by $t_2 - t_1$, and denoting the time average by a bar,

$$\lim_{\substack{t_2\to\infty \\ t_1\to -\infty}} \frac{1}{t_2 - t_1}[\quad]_{t_1}^{t_2} = \alpha \bar{L}\,. \tag{6}$$

This equation has the form of a virial theorem applicable to any solution $q_k(t)$ for which the limit exists.

Remark. Suppose that one knows *two* different infinitesimal transformations, for each of which (5) holds, with suitable α_1, α_2. They can then be combined to give one transformation having $\alpha = 0$, and one other transformation obeying (5). The former yields a constant of the motion and the latter yields a virial theorem. Hence no system can have more than a single independent virial theorem.

6. Equation (6) is too general for most applications. We therefore first suppose that $L(q, \dot{q})$ does not contain t as an explicit variable. In that case the energy

$$E(q\,,\dot{q}) = \frac{\partial L}{\partial \dot{q}_k}\,\dot{q}_k - L$$

is a constant of the motion. Hence (6) may be written

$$\frac{1}{t_2 - t_1}\left[\frac{\partial L}{\partial \dot{q}_k}\,\chi_k - \Omega\right]_{t_1}^{t_2} - \frac{E}{t_2 - t_1}\,[\varphi]_{t_1}^{t_2} = \alpha\bar{L}\,, \tag{7}$$

the limit being understood.

Next we suppose that the relevant transformation is simply a scale transformation,

$$\varphi(t\,, q) = \beta t\,, \qquad \chi_k(t\,, q) = q_k\,, \tag{8}$$

and that $\Omega = 0$. This turns out to cover all familiar applications. Equation (7) now reduces to

$$\frac{1}{t_2 - t_1}\,[p_k\,q_k]_{t_1}^{t_2} - \beta E = \alpha\bar{L}\,. \tag{9}$$

One readily finds from this the well-known results for the harmonic oscillator ($\beta = 0$, $\alpha = 2$) and the Kepler motion ($\beta = \frac{3}{2}$, $\alpha = \frac{1}{2}$).

7. The following is a slightly less familiar example. The Lagrange function for a charged particle in a magnetic field is

$$L(\boldsymbol{r}\,, \dot{\boldsymbol{r}}) = \tfrac{1}{2}m\dot{\boldsymbol{r}}^2 + e\dot{\boldsymbol{r}}\cdot\boldsymbol{A}(\boldsymbol{r})\,.$$

Let the vector potential $A(r)$ be a homogeneous polynomial of degree μ in the coordinates. Then the scale transformation (8) with $\beta=1-\mu$ obeys (9) with $\alpha=1+\mu$. The result is

$$\frac{1}{t_2-t_1}\,[p\cdot r]_{t_1}^{t_2}-m\overline{\dot{r}^2}=(1+\mu)\,\overline{e\dot{r}\cdot A(r)}\,.$$

For any solution that is bounded in space one has therefore

$$-\frac{m}{1+\mu}\,v=e\,\overline{A(r)\cos\vartheta}\,,$$

where v is the constant velocity, and ϑ its angle with the direction of $A(r)$. An alternative way of putting it is

$$e\int_0^T A(r)\cdot dr+\frac{2}{1+\mu}\,ET=O(1)$$

as $T\to\infty$.

8. The application of the virial theorem is not confined to cases in which the first term in (9) vanishes. This is well known from the familiar application to gases, and is also demonstrated by the following example from scattering theory. The Lagrange function for a particle under influence of a repulsive potential $V(r)=Cr^{-\mu}$ $(\mu>1)$ is

$$L(r,\dot{r})=\frac{m}{2}\,\dot{r}^2-Cr^{-\mu}.$$

This L obeys (5) with

$$\varphi=(1+\tfrac{1}{2}\mu)\,t\,,\qquad \chi=r\,,\qquad \alpha=1-\tfrac{1}{2}\mu\,,\qquad \Omega=0\,.$$

According to (9)

$$m\left[\dot{r}\cdot r\right]_{t_1}^{t_2}-(1+\tfrac{1}{2}\mu)\,E\,(t_2-t_1)=(1-\tfrac{1}{2}\mu)\int_{t_1}^{t_2}L\,dt\,. \tag{10}$$

The free motion at large distance is described by

$$r=\underline{v}(t-\tau)+b\,,\qquad (\underline{v}\cdot b)=0\,, \tag{11}$$

with constants $\underline{v}_1,\tau_1,b_1$ for the incoming particle and $\underline{v}_2,\tau_2,b_2$ for the outgoing particle. One has $v_1^2=v_2^2=2E/m$, while $\tau_2-\tau_1$ is the delay due to the interaction, i.e., the delay as compared to a particle that would move with constant velocity $\underline{v}_1$ into the origin and from there with velocity $\underline{v}_2$ in the scattered direction. Substituting (11) in the first term of (10) one finds

$$2E(\tau_2-\tau_1)=(2-\mu)\int_{-\infty}^{\infty}V\,dt\,,$$

or alternatively

$$2E(\tau_2 - \tau_1) = (2-\mu) \int\limits_{-\infty}^{\infty} \frac{V}{\sqrt{2(E-V)/m}}\, ds .$$

This expresses the delay in terms of an integral along the actual path.

The potential $V(r) = Cr^{-2}$ has the property that the delay always vanishes. This result may be verified explicitly and can also be shown to be true for a nonrelativistic Schrödinger particle.

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