Zeitschrift: Helvetica Physica Acta

Band: 53 (1980)

Heft: 3

Artikel: The virial theorem in four branches of physics and its derivation

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DOI: https://doi.org/10.5169/seals-115132

Helvetica Physica Acta, Vol. 53 (1980), Birkhäuser Verlag, Basel

The virial theorem in four branches of physics and its derivation[1])

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(1. IX. 1980; rev. 7. XI. 1980)

Abstract. A generalized version of the virial theorem is proved in classical mechanics, classical statistical mechanics, quantum mechanics and quantum statistics.

1. Introduction

With a few exceptions, realistic physical dynamical systems cannot be integrated explicitly. Global information on the dynamical behaviour of the system is therefore of great interest. The existence of constants of the motion and stability criteria are famous examples thereof. Another example we will deal with here is the virial theorem.

In the textbooks usually different and separate discussions of the virial theorem in classical mechanics, statistical mechanics, quantum mechanics, and in quantum statistics are given. This prevents a clear vision of the virial theorem, its difference and similarity in the different branches of physics. Furthermore, in our opinion most discussions are not very transparent. Consequently, the simplicity and elegance of the virial theorem remains hidden.

For a general classical system of n mass points with position vectors $\mathbf{r}_i$ and applied forces $\mathbf{F}_i$ (including any forces of constraints), the virial theorem is usually formulated as (e.g. Goldstein [1])

$$\langle T\rangle = -\frac{1}{2}\left\langle \sum_{i=1}^{n} \mathbf{F}_i \cdot \mathbf{r}_i \right\rangle. \tag{1.1}$$

Here T is the kinetic energy

$$T = \sum_{i=1}^{n} \tfrac{1}{2} m_i \dot{\mathbf{r}}_i \cdot \dot{\mathbf{r}}_i \tag{1.2}$$

and the angular brackets denote time averages:

$$\langle g\rangle = \lim_{t_{1,2}\to\mp\infty} \frac{1}{t_2 - t_1} \int_{t_1}^{t_2} g\, dt \tag{1.3}$$

The right-hand side of (1.1) is called the *virial of Clausius.*

[1]) Work supported by the Swiss National Science Foundation

The theorem is very useful in the kinetic theory of gases. Only a few further steps are required to prove Boyle's law for perfect gases (e.g. Lindsay [2]). It is practically indispensable for calculating the equations of state for imperfect gases, where the forces $\mathbf{F}_i$ include not only the forces of constraint keeping the gas particles inside the container but also the interaction forces between molecules (e.g. Kittel [3], Wilson [4]). Other possible applications of the virial theorem are its use as a method to ascertain the accuracy of approximate solutions [5] and its use in optimizing a parameter in a trial function of an (approximate) solution. E.g. approximations for the frequency of an anharmonic oscillator are found easily [6].

For Hamiltonian systems described by the Hamiltonian H as a function of the coordinates $q_1, q_2, \ldots, q_N$ and momenta $p_1, p_2, \ldots, p_N$, the virial theorem (1.1) takes the form

$$\left\langle \sum_{i=1}^{N} q_i \frac{\partial H}{\partial q_i} \right\rangle = \left\langle \sum_{i=1}^{N} p_i \frac{\partial H}{\partial p_i} \right\rangle. \tag{1.4}$$

A generalization that has been discussed elsewhere [7] reads: For arbitrary but bounded $f(q_1, \ldots, q_N, p_1, \ldots, p_N)$ the following identity holds

$$\left\langle \sum_{i=1}^{N} \frac{\partial f}{\partial q_i} \frac{\partial H}{\partial p_i} \right\rangle = \left\langle \sum_{i=1}^{N} \frac{\partial f}{\partial p_i} \frac{\partial H}{\partial q_i} \right\rangle. \tag{1.5}$$

With $f = \sum_{i=1}^{N} p_i q_i$, equation (1.5) yields the usual virial theorem (1.4).

The usual virial theorem (1.1) or (1.4) of classical mechanics is also valid in classical statistical mechanics [8], [9], in quantum mechanics [5], [10] and in quantum statistics, if statistical ensemble averages, quantum mechanical expectation values and quantum statistical ensemble averages, respectively, are substituted for classical time averages.

In this paper the generalized virial theorem both in classical mechanics, in classical statistical mechanics, in quantum mechanics and in quantum statistics will be derived. In contrast with some other authors, e.g. van Kampen [11] and Miglietta [12], who derive modifications of the virial theorem with symmetry methods, in this paper the virial theorem is derived by means of the equations of motion only. As a result the derivations of this important theorem become almost trivial, which is the main pedagogical advantage of the present approach.

2. Classical mechanics

Let the observable $f(p, q)$ be a function of the canonical variables $p_1, p_2, \ldots, p_n, q_1, \ldots, q_n$. Then from Hamilton's equations of motion it follows that

$$d/dt\, f = [f, H] = \sum_{i=1}^{n} \left(\frac{\partial f}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial H}{\partial q_i} \right), \tag{2.1}$$

where the square brackets are the Poisson brackets. If f is assumed to be bounded in time for all possible solutions $p_i(t)$, $q_i(t)$, the time average $\langle d/dt\, f \rangle$ of $d/dt\, f$ reads

$$\langle d/dt\, f \rangle = \lim_{\substack{t_1 \to -\infty \\ t_2 \to \infty}} \frac{1}{t_2 - t_1} \int_{t_1}^{t_2} d/dt\, f = 0. \tag{2.2}$$

From (2.1) and (2.2) then follows for any $f(p, q)$ which is bounded in time

$$\left\langle \sum_i \frac{\partial f}{\partial q_i} \frac{\partial H}{\partial p_i} \right\rangle = \left\langle \sum_i \frac{\partial f}{\partial p_i} \frac{\partial H}{\partial q_i} \right\rangle, \tag{2.3}$$

which is the virial theorem in classical mechanics.

3. Classical statistical mechanics

The underlying theory of classical statistical mechanics is classical mechanics. Thus, for any $f(p, q)$ equation (2.1) is still valid. The statistical average $\langle A \rangle$ of some observable $A(p, q)$ is defined as an integral over phase space

$$\langle A \rangle = \int \rho(H(p, q)) A(p, q)\, d^n p\, d^n q, \tag{3.1}$$

where $\rho(H)$ is the canonical or micro canonical density function on phase space. The combination of (2.1) and (3.1) yields

$$\langle d/dt\, f \rangle = \left\langle \sum_{i=1}^{n} \left(\frac{\partial f}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial H}{\partial q_i} \right) \right\rangle = \int \rho(H(p, q)) \sum_{i=1}^{n} \left(\frac{\partial f}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial H}{\partial q_i} \right) d^n p\, d^n q \tag{3.2}$$

Let now $\rho(H) = d/dH\, R(H)$, then with the condition

$$R(H(p, q)) \frac{\partial f}{\partial p_i} \to 0, \qquad R(H(p, q)) \frac{\partial f}{\partial q_i} \to 0 \quad \text{for} \quad p, q \to \pm\infty \tag{3.4}$$

an integration by parts gives

$$\int \rho(H(p, q)) \sum_{i=1}^{n} \frac{\partial f}{\partial q_i} \frac{\partial H}{\partial p_i}\, d^n p\, d^n q = \int \rho(H(p, q)) \sum_{i=1}^{n} \frac{\partial f}{\partial p_i} \frac{\partial H}{\partial q_i}\, d^n p\, d^n q$$

$$= - \int \sum_{i=1}^{n} \frac{\partial^2 f}{\partial p_i \partial q_i} R(H(p, q))\, d^n p\, d^n q. \tag{3.5}$$

Together with (3.1) this yields (2.3) again, but now with the condition (3.4) and the angular brackets interpreted as statistical averages. This we call the virial theorem for classical statistical mechanics. Let us investigate the condition (3.4) for the canonical and the microcanonical ensemble separately.

The canonical ensemble is defined by

$$\rho(H) = \exp -\beta H, \tag{3.6}$$

where

$$\beta = 1/kT. \tag{3.7}$$

Then suitable integration constants give

$$R(H) = -1/\beta \exp -\beta H, \tag{3.8}$$

and the condition (3.4) reads

$$\frac{\partial f}{\partial q_i}\exp -\beta H \to 0, \qquad \frac{\partial f}{\partial p_i}\exp -\beta H \to 0, \tag{3.9}$$

for $p, q \to \pm\infty$.

Systems usually discussed in statistical mechanics are contained within a container. The forces of constraint keeping the system within the container can be described assuming an infinite potential energy outside the container. Then $H \to \infty$ for $q \to \pm\infty$. Furthermore the kinetic energy part of H goes to infinity for $p \to \pm\infty$. So, for such systems the condition (3.9) is satisfied automatically. The micro- canonical ensemble is described by

$$\rho(H) = \delta(E_0 - H), \tag{3.10}$$

which with suitable integration constants yields

$$\begin{aligned} R(H) &= \ \ 0 \qquad (H > E_0) \\ &= -1 \qquad (H < E_0), \end{aligned} \tag{3.11}$$

Thus also in this case the condition (3.4) is satisfied automatically as long as $H > E_0$ for $p, q \to \pm\infty$.

4. Quantum mechanics

In quantum mechanics, an observable $f(p, q)$ is a Hermitean operator which works in a Hilbert space and which depends on the Hermitean momentum and position operators p_i and q_i $(i = 1, 2, \ldots, n)$. Within Heisenberg's picture, the dynamics of an observable is given by

$$d/dt\, f(p, q) = [f, H] = \frac{1}{i\hbar}(fH - Hf), \tag{4.1}$$

where H is the Hamilton operator, $\hbar$ is Dirac's constant and the square brackets now stay for $1/i\hbar$ times the commutator. In the appendix it is shown that when either f or H is a polynomial in p and q of second degree and with real coefficients, the following identity holds

$$[f, H] = \frac{1}{2}\sum_{i=1}^{n}\left(\frac{\partial f}{\partial q_i}\frac{\partial H}{\partial p_i} + \frac{\partial H}{\partial p_i}\frac{\partial f}{\partial q_i}\right) - \frac{1}{2}\sum_{i=1}^{n}\left(\frac{\partial f}{\partial p_i}\frac{\partial H}{\partial q_i} + \frac{\partial H}{\partial q_i}\frac{\partial f}{\partial p_i}\right) \tag{4.2}$$

The quantum mechanical average (expectation value) $\langle A\rangle$ of some observable A, in some state $|\psi\rangle$ is

$$\langle A\rangle = \langle\psi|\, A\, |\psi\rangle. \tag{4.3}$$

Under the assumption that $|\psi\rangle$ represents a stationary state with energy E

$$H\,|\psi\rangle = E\,|\psi\rangle \tag{4.4}$$

holds. Then with (4.1) and (4.4)

$$\begin{aligned} i\hbar\langle d/dt\, f\rangle &= \langle\psi|\, [f, H]\, |\psi\rangle = \langle\psi|\, fH - Hf\, |\psi\rangle \\ &= \langle\psi|\, fE - Ef\, |\psi\rangle = 0 \end{aligned} \tag{4.5}$$

Equations (4.2) and (4.5) together yield

$$\left\langle \sum_{i=1}^{n} \left(\frac{\partial f}{\partial q_i} \frac{\partial H}{\partial p_i} + \frac{\partial H}{\partial p_i} \frac{\partial f}{\partial q_i} \right) \right\rangle = \left\langle \sum_{i=1}^{n} \left(\frac{\partial f}{\partial p_i} \frac{\partial H}{\partial q_i} + \frac{\partial H}{\partial q_i} \frac{\partial f}{\partial p_i} \right) \right\rangle, \tag{4.6}$$

which holds for either H or f a polynomial in p and q of second degree and real coefficients and the angular brackets denoting the quantum mechanical expectation value. This is the quantum mechanical version of the virial theorem for a system in a stationary state.

We stress that the above formulation of the virial theorem implies the essential restriction of either f or H being polynomials in p and q of second degree. So, for arbitrary Hamiltonians, equation (4.6) is only valid for f being a polynomial in p and q of degree two.

5. Quantum Statistics

The underlying theory of quantum statistics is quantum mechanics. Thus also equation (4.2) holds if either f or H depend maximally quadratic on p and q. Furthermore, in quantum statistics, the statistical average $\langle A \rangle$ of some observable $A(p, q)$ is

$$\langle A \rangle = \mathrm{Tr}\, \rho A, \tag{5.1}$$

where ρ is the equilibrium statistical density operator that depends on integrals of the motion only. Therefore, ρ commutes with H:

$$\rho H = H\rho. \tag{5.2}$$

Then with (4.1)

$$\begin{aligned} \langle d/dt\, f \rangle &= 1/\hbar \langle [f, H] \rangle = 1/i\hbar\, \mathrm{Tr}\,(\rho f H - \rho H f) \\ &= 1/i\hbar\, \mathrm{Tr}\,(H\rho f - H\rho f) = 0. \end{aligned} \tag{5.3}$$

Equation (4.2) and (5.3) together yield

$$\left\langle \sum_{i=1}^{n} \left(\frac{\partial f}{\partial q_i} \frac{\partial H}{\partial p_i} + \frac{\partial H}{\partial p_i} \frac{\partial f}{\partial q_i} \right) \right\rangle = \left\langle \sum_{i=1}^{n} \left(\frac{\partial f}{\partial p_i} \frac{\partial H}{\partial q_i} + \frac{\partial H}{\partial q_i} \frac{\partial f}{\partial p_i} \right) \right\rangle. \tag{5.4}$$

Thus, also in the interpretation of the angular brackets as quantum statistical averages, equation (4.6) holds if either f or H is a polynomial in p and q of second degree and with real coefficients. This is the quantum statistical version of the virial theorem.

6. Discussion

The undeniable importance of the virial theorem seems to contradict its extreme simplicity. Therefore one might be lured into looking for connections of the virial theorem with other properties of the system, and thus expecting a deeper understanding of the virial theorem. For an example the reader is referred to the recent paper of Kleban [13], in which a special form of the virial theorem, that is equivalent to our equation (1.4), is related to scale transformations.

Any function $f(p, q)$ on phase space can be considered as the generating function of a one-parametric family of canonical transformations (e.g. see Rosen [14])

$$p_i \to p_i^s = p_i^s(p, q); \qquad q_i \to q_i^s = q_i^s(p, q). \tag{6.1}$$

such that

$$d/ds\, p_i^s = [p_i^s, f], \qquad d/ds\, q_i^s = [q_i^s, f] \tag{6.2}$$

and $p_i^0 = p_i$, $q_i^0 = q_i$. The transform $g^s(p, q)$ of some function $g(p, q)$ is then defined as

$$g^s(p, q) = g(p^s(p, q), q^s(p, q)) \tag{6.4}$$

such that also

$$d/ds\, g^s = [g^s, f], \qquad g^0 = g. \tag{6.5}$$

For instance replacement of $g(p, q)$ by the Hamiltonian $H(p, q)$ gives

$$d/ds\, H^s = [H^s, f], \qquad H^0 = H \tag{6.6}$$

such that

$$(d/ds\, H^s)_{s=0} = [H, f] = -[f, H] \tag{6.7}$$

or

$$(d/ds\, H^s)_{s=0} = -d/dt\, f. \tag{6.8}$$

This relation, applied to $f = \sum p_i q_i$ and restricted to infinitesimal transformations is the central result of Kleban's paper. Indeed for $f = \sum p_i q_i$, integrating equations (6.2)–(6.3) yields the scale transformation

$$p_i^s = p_i e^{-s}, \qquad q_i^s = q_i e^s.$$

The relation between this piece of transformation theory, and the virial theorem is only the fact that both use some function f. Therefore we do not see any pedagogical advantage or any other reason to drag in transformation theory in the discussion of the virial theorem. In classical mechanics, the virial theorem is equivalent to the trivial statement 'The time average of the time-derivative of a bounded function is zero'. This trivially does not detract anything from the importance of the virial theorem.

Appendix

In classical mechanics, the symplectic formalism is introduced by setting $(x_1, x_2, \ldots, x_{2n}) = (q_1, q_2, \ldots, q_n, p_1, \ldots, p_n)$. Then the Poisson bracket $[f, g]$ can be written as

$$[f, g] = \omega_{ij} \frac{\partial f}{\partial x_i} \frac{\partial g}{\partial x_j}, \tag{A1}$$

where a summation of the repeated indices is assumed from 1 through $2n$, and ω_{ij} is given by

$$\omega_{ij} = \delta_{i+n,j} (0 < i \leq n), \qquad \omega_{ij} = -\delta_{i,j+n} (n < i \leq 2n) \tag{A2}$$

and δ_{ij} is the usual Kronecker delta symbol. Then

$$\omega_{ij} = -\omega_{ji}; \qquad \omega_{ij}\omega_{ik} = \omega_{ji}\omega_{ki} = -\omega_{ji}\omega_{ik} = \delta_{jk}, \tag{A3}$$

$$[x_i, x_j] = \omega_{ij} \tag{A4}$$

and

$$\frac{\partial g}{\partial x_i} = \omega_{ij}[x_i, g]. \tag{A5}$$

In quantum mechanics, the square brackets denote the commutator:

$$[f, g] = \frac{1}{i\hbar}(fg - gf) \tag{A6}$$

Then with (A2) still (A4) is true and (A5) can be considered as the definition of the operator $\partial/\partial x_j$. Now let $f(x)$ be a polynomial in p and q, of second degree, i.e. $f(x)$ takes the form

$$f = c + \alpha_i x_i + \gamma_{ij} x_i x_j \tag{A7}$$

where c, α_i and γ_{ij} are constants. Then $[f, g]$ is easily calculated:

$$\begin{aligned}[f, g] &= [c + \alpha_i x_i + \gamma_{ij} x_i x_j, g] \\ &= \alpha_i [x_i, g] + \gamma_{ij}[x_i, g]x_j + \gamma_{ij} x_i [x_j, g].\end{aligned} \tag{A8}$$

On the other hand,

$$\begin{aligned}\frac{\partial f}{\partial x_k} &= \omega_{lk}[x_l, f] = \omega_{kl}[f, x_l] \\ &= \omega_{kl}[c + \alpha_i x_i + \gamma_{ij} x_i x_j, x_l] \\ &= \alpha_i \omega_{kl}\omega_{il} + \gamma_{ij}\omega_{kl}\omega_{jl} x_i + \gamma_{ij}\omega_{kl}\omega_{il} x_j \\ &= \alpha_k + (\gamma_{jk} + \gamma_{kj}) x_j\end{aligned} \tag{A9}$$

Consequently with (A5)

$$\tfrac{1}{2}\omega_{kl}\left(\frac{\partial f}{\partial x_k}\frac{\partial g}{\partial x_l} + \frac{\partial g}{\partial x_l}\frac{\partial f}{\partial x_k}\right) = \alpha_i[x_i, g] + \tfrac{1}{2}(\gamma_{ij} + \gamma_{ji})([x_i, g]x_j + x_j[x_i, g]). \tag{A10}$$

In quantum mechanics the extra condition

$$\gamma_{ij} = \gamma_{ji}, \tag{A11}$$

yields

$$[f, g] = \tfrac{1}{2}\omega_{kl}\left(\frac{\partial f}{\partial x_k}\frac{\partial g}{\partial x_l} + \frac{\partial g}{\partial x_l}\frac{\partial f}{\partial x_k}\right). \tag{A12}$$

Abandonment of the symplectic notation gives

$$[f, g] = \sum_{i=1}^{n} \left[\frac{1}{2}\left(\frac{\partial f}{\partial q_i}\frac{\partial g}{\partial p_i} + \frac{\partial g}{\partial p_i}\frac{\partial f}{\partial q_i}\right) - \frac{1}{2}\left(\frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q_i} + \frac{\partial g}{\partial q_i}\frac{\partial f}{\partial p_i}\right)\right] \tag{A11}$$

which is true for either f or g of the form (A7) with condition (A11).

The operators representing physical quantities are Hermitean. Therefore, one easily sees from (A7) that we must have

$$\gamma_{ij} = \gamma_{ij}^*, \qquad \alpha_i = \alpha_i^*, \qquad c = c^*. \tag{A14}$$

Together with (A11) this means that all coefficients in (A7) are real. Thus, (A13) is true for both f and g Hermitean operators and either f or g a polynomial in q and p of second degree and with real coefficients.

Acknowledgement

The author would like to thank A. Thellung for stimulating discussions which have lead to this paper, and for his criticism of the final text.

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