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Groups of canonical transformations and the virial-Noether theorem

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Abstract. *In Hamiltonian mechanics a characterization of the infinitesimal generator of one-parameter Lie Groups of non-univalent canonical transformations is given. The result is used to derive a general form of the virial theorem, which has Noether's theorem as a special case. The theory is applied to the Toda lattice system.*

1. INTRODUCTION

A basic strategy in dealing with classical mechanics is looking for integrals of the motion. This theory started with the notion of cyclic coordinates and culminated in Noether's fundamental theorem [1], which associates to each one-parameter group of symmetry transformations of the Hamiltonian an integral of the motion.

Another result in classical mechanics relevant for physical applications is the virial theorem. In textbooks this theorem appears as a result independent from the theory of constants of the motion. However in [2] van Kampen gave a derivation of the virial theorem based on the idea that it is a consequence of the form invariance of the equations of motion under a continuous transformation. It is

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well-known that form invariance of the equations of motion does not imply necessarily a symmetry transformation of the system.

In this paper we work out this idea for Hamiltonian mechanics on symplectic manifolds. In section II we study one-parameter Lie groups of transformations leaving the symplectic structure form invariant, but not strictly invariant, i.e. the canonical two-form is transformed into a multiple of itself. It can be shown that this property is equivalent to form invariance of the equations of motion [3]. In particular we give a complete characterization of the infinitesimal generator of such one-parameter groups and prove that it is given by a linear combination of a Hamiltonian vector field and the infinitesimal generator of the dilations. The usual proof of the virial theorem is based on the study of the time evolution of the infinitesimal generator of the dilations. Therefore our one-parameter groups of canonical transformations are genuinely connected to the virial theorem. In section III we use our results to derive a very general form of the virial theorem, which has Noether's theorem as a special case.

Finally, we conclude by a detailed application of the virial theorem to the Toda lattice system. Contrary to the familiar applications of this theorem where only scale transformations are used, in this model we go beyond them and employ a combined scale-translation transformation group, illustrating the power of the method.

II. ONE-PARAMETER GROUPS OF NON-UNIVALENT CANONICAL TRANSFORMATIONS

Let Γ be the classical phase space which as usual is an even dimensional analytic manifold. We consider Γ to be equipped with a symplectic structure given by a closed nondegenerate analytic 2-form ω^2, i.e. ω^2 satisfies: $d\omega^2 = 0$ and for any $\xi \in T\Gamma_x$, the tangent space at the point x of $\Gamma : \omega^2(\xi, \eta) = 0$ for all $\eta \in T\Gamma_x$ implies $\xi = 0$. Therefore the phase space Γ is a symplectic analytic manifold.

Furthermore, we suppose that there exists an analytic 1-form ω^1 such that $\omega^2 = d\omega^1$, or a vectorfield X_1 for which $d\, i_{X_1}\omega^2 = \omega^2$; $i_{X_1}\omega^2$ is the inner product of X_1 and ω^2.

As an example take $\Gamma = \mathbb{R}^2$ with the chart (q, p), then a natural symplectic structure is given by the 2-form $\omega^2 = dq \wedge dp$ and the corresponding 1-form by $\omega^1 = -p\, dq$, or $X_1 = -p\,\partial/\partial p$.

Next we introduce the notion of canonical transformation.

Consider g an analytic one-to-one mapping of the phase space Γ into itself. This mapping defines a linear map of the tangent spaces which, in turn, introduces the map g^* of the analytic k-forms.

DEFINITION II.1. A mapping g, as described above, such that there exists a non zero constant $c \in \mathbb{R}$, satisfying

$$g^{*}\omega^{2} = c\omega^{2} \tag{1}$$

is called a *canonical transformation of valence c*. ■

Denote by K the set of canonical transformations. It is clear that K is a group for the composition law of successive application of the transformations. Remark that the set K_1 of canonical transformations for which $c = 1$ in (1) is a non trivial subgroup of K; K_1 is called the group of univalent canonical transformations, leaving the 2-form ω^2 invariant. Most authors [4 - 7] restrict themselves to this set of univalent canonical transformations.

For what follows it is important to notice that we study the extended group K of canonical transformations [8]. As is clear from the definition they do not leave, in the strict sense of the word, the 2-form ω^2 invariant, but it can be shown that the elements of K do preserve the structure of the Hamilton canonical equations of motion [3].

Next we introduce a 1-parameter Lie group G, a subgroup of the group K of canonical transformations. Denote by $\lambda \in \mathbb{R}$ the canonical chart of the Lie group G, i.e. for each $\lambda_1, \lambda_2 \in \mathbb{R}$ there exists $g(\lambda_1), g(\lambda_2) \in G$ such that

$$g(\lambda_1)\, g(\lambda_2) = g(\lambda_1 + \lambda_2)$$

Denote by $c(\lambda)$ the valence of the canonical transformation $g(\lambda)$ element of G, then the function $c : \lambda \in \mathbb{R} \to c(\lambda) \in \mathbb{R}$ is analytic and from (1) it follows that

$$c(\lambda_1)\, c(\lambda_2) = c(\lambda_1 + \lambda_2).$$

Hence, there exists a constant $a \in \mathbb{R}$ such that

$$c(\lambda) = \exp a\lambda. \tag{2}$$

The case $a = 0$ reduces to $G \subset K_1$.

Denote by $A(\Gamma)$ the set of analytic functions on the phase space Γ, then the Lie algebra of G is generated by the vectorfield X defined by

$$(Xf)(x) = \left.\frac{\mathrm{d}f(g(\lambda)x)}{\mathrm{d}\lambda}\right|_{\lambda=0}. \tag{3}$$

The components of X are then $X^i = Xx^i$.

THEOREM II.2. *Let* $G = \{g(\lambda)\}_{\lambda \in \mathbb{R}}$ *be a 1-parameter Lie group of canonical transformations of the symplectic analytic manifold* Γ, *equipped with the 2-*

-form ω^2. *Let* X_1 *be a vectorfield such that* $\omega^2 = \mathrm{d}\, i_{X_1} \omega^2$ *then there exists locally a function* $\phi \in A(\Gamma)$ *such that with* X *the vector field of* G *one has:*

$$\mathrm{d}\phi = i_X \omega^2 - a\, i_{X_1} \omega^2 \tag{4}$$

where the constant a *is defined in* (2).

Proof. Using definition II.1, formula (2) and $\omega^2 = \mathrm{d}\, i_{X_1} \omega^2$

$$a\omega^2 = \left.\frac{\mathrm{d}(g^*(\lambda)\omega^2)}{\mathrm{d}\lambda}\right|_{\lambda=0} = \mathrm{d} \left.\frac{\mathrm{d}(g^*(\lambda)\, i_{X_1} \omega^2)}{\mathrm{d}\lambda}\right|_{\lambda=0} .$$

Applying Thm 2.4.13 of [5] for $i_{X_1} \omega^2$:

$$\left(\frac{\mathrm{d}\, g^*(\lambda)\, i_{X_1} \omega^2}{\mathrm{d}\lambda}\right)_{\lambda=0} = i_X\, \mathrm{d}\, i_{X_1} \omega^2 + \mathrm{d}\, i_X i_{X_1} \omega^2$$

hence

$$\mathrm{d}(a\, i_{X_1} \omega^2 - i_X \omega^2) = 0$$

yielding the result. ∎

By means of this theorem the generator X of the Lie group G is expressed in terms of the function ϕ. Due to the non-degeneracy of ω^2 formula (4) defines X uniquely. The vectorfield X depends only on ω^2. Formula (4) can be viewed as the defining relation of ϕ. The latter one depends on the vector fields X and X_1.

Now we are interested in the inverse question, namely whether each vectorfield X defined by equation (4) generates a 1-parameter Lie group of canonical transformations. The answer is in the following theorem, which we formulate in the case ϕ is globally given. If ϕ is only locally given one gets only a local group.

THEOREM II.3. *Suppose* $\phi \in A(\Gamma)$ *be given, where* Γ *is again the symplectic manifold with the 2-form* ω^2 *and the vector field* X_1 *such that* $\mathrm{d}\, i_{X_1} \omega^2 = \omega^2$, *then the vectorfield* X *defined by equation* (4), *generates a* 1*-parameter Lie group* $G = \{g(\lambda)\}_{\lambda \in \mathbb{R}}$ *of canonical transformations with the group of valences* $\{c(\lambda) = \exp a\lambda\}_{\lambda \in \mathbb{R}}$.

Proof. Define the map $g(\lambda)$ of Γ by:

$$g(\lambda) : x \in \Gamma \to g(\lambda)\, x \in \Gamma$$

such that for fixed $x \in \Gamma$, $\lambda \to g(\lambda)\, x$ is the unique solution with initial values $x = g(0)x$, of the first order differential equations

$$\frac{\partial (g(\lambda)x)^i}{\partial \lambda} = X(g(\lambda)x)^i; \qquad (i = 1, \ldots, 2n).$$

It is wellknown (see e.g. [9, Theorems 6.2.1 and 3.5.2]) that $G = \{g(\lambda)\}_{\lambda \in \mathbb{R}}$ is a 1-parameter Lie group and λ is a canonical chart: $g(\lambda_1)\, g(\lambda_2) = g(\lambda_1 + \lambda_2)$; λ_1, $\lambda_2 \in \mathbb{R}$. Next we check that for each $\lambda \in \mathbb{R}$, $g(\lambda)$ is a canonical transformation. Using Thm 2.4.13 of [5] and the fact that ω^2 is closed

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\, g^\star(\lambda)\omega^2 = g^\star(\lambda)(i_X\, \mathrm{d}\omega^2 + \mathrm{d}(i_X \omega^2)) = g^\star(\lambda)\, \mathrm{d}(i_X \omega^2).$$

Using formula (4):

$$0 = \mathrm{d}^2 \phi = \mathrm{d}(i_X \omega^2) - a\omega^2.$$

Hence

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\, g^\star(\lambda)\omega^2 = a\, g(\lambda)\omega^2$$

and therefore, as $g^\star(0)$ is the identity map:

$$g^\star(\lambda)\omega^2 = e^{a\lambda}\omega^2$$

proving (1). This concludes the proof of the Theorem. ∎

It is instructive to specialize to the case that Γ has a local chart $(q^1, \ldots, q^n, p^1, \ldots, p^n)$ and locally

$$\omega^2 = \sum_i \mathrm{d}q^i \wedge \mathrm{d}p^i \tag{5}$$

one can choose for X_1 the following vectorfield:

$$X_1 = \frac{1}{2} \sum_i \left(q^i \frac{\partial}{\partial q^i} - p^i \frac{\partial}{\partial p^i} \right) \tag{6}$$

then one has the solution of (4)

$$X = [\ .\ , \phi] + a\, X_1$$

where the bracket

$$[f, g] = \sum_i \frac{\partial f}{\partial q^i}\,\frac{\partial g}{\partial p^i} - \frac{\partial f}{\partial p^i}\,\frac{\partial g}{\partial q^i}$$

mapping $A(\Gamma) \times A(\Gamma)$ in $A(\Gamma)$, is the usual Poisson bracket.

In the case of univalent canonical transformations ($a = 0$) this formula reduces to the wellknown statement that the generator of 1-parameter groups of canonical transformations is given by the Poisson bracket with a function, in other words the generators are Hamiltonian vector fields. Here we see that for general 1-parameter groups of canonical transformations the generator is given by the sum of a Hamiltonian vectorfield and a vectorfield X_1, which is a generator of dilations.

III. THE VIRIAL-NOETHER THEOREM AND APPLICATIONS

Let us first introduce a Hamiltonian system with Hamiltonan $H:(q,p) \in \Gamma \to H(q,p) \in \mathbb{R}$ such that $H \in A(\Gamma)$.

The canonical equations of motion are then

$$\dot{f} = [f, H], \quad f \in A(\Gamma) \tag{7}$$

with solution $f_t(q_0, p_0)$; $q_0 = q(t_0)$, $p_0 = p(t_0)$ initial values. The preceeding characterization of the generators of 1-parameter Lie groups of canonical transformations is now used to derive a generalization of Noether's theorem. Here we consider 1-parameter groups of transformations which do not leave necessarily the Hamiltonian invariant, as they do in Noether's theorem, but which transform it in a trivial way in the sense that they multiply it by a constant. The result we get is the virial theorem, yielding as a special case Noether's theorem.

Let $G = \{g(\lambda)\}_{\lambda \in \mathbb{R}}$ be a one-parameter Lie group of canonical transformations of the symplectic manifold Γ, equipped with ω^2 and X_1 as above. Then there exists a function $\phi \in A(\Gamma)$ such that

$$[H, \phi] + a\,X_1 H = \left.\frac{\mathrm{d}(g^*(\lambda)H)}{\mathrm{d}\lambda}\right|_{\lambda=0} \tag{8}$$

In particular, if $g^*(\lambda)\,H = (\exp b\lambda)\,H$, with $b \in \mathbb{R}$ then

$$[H, \phi] + a\,X_1 H = b\,H. \tag{9}$$

Remark that one recovers Noether's theorem in the case $a = b = 0$. Furthermore, if the Hamiltonian H takes the usual form

$$H(q,p) = T(p) + V(q)$$

with $T(p)$ the kinetic energy and $V(q)$ the potential energy, then

$$\left[V(q), \sum_i p^i q^i\right] = \sum_i q^i \frac{\partial V(q)}{\partial q^i}$$

which is known in the literature as the virial of the system.

For Hamiltonians H which have a Legendre transform L with respect to the conjugate momenta p i.e. if

$$\det\left(\frac{\partial^2 H}{\partial p^i \partial p^j}\right) \neq 0$$

we have the Lagrangian:

$$L(q, \dot{q}) = \sum_{i=1}^{n} p^i \dot{q}^i - H(q, p)$$

and $2T = L + H$.

Take ω^2 and X_1 as in (5) and (6), then

$$X_1 H = \frac{1}{2}\left[H, \sum_i p^i q^i\right] + 2T \tag{10}$$

therefore (8) and (9) become

$$\left[H, \phi + \frac{a}{2} \sum_i q^i p^i\right] + 2T = \left.\frac{d(g^*(\lambda)H)}{d\lambda}\right|_{\lambda=0} \tag{11}$$

$$\left[H, \phi + \frac{a}{2} \sum_i q^i p^i\right] + 2T = bH. \tag{12}$$

If one has additional information about the system one can derive more conclusions. Here we limit ourselves to a result which is frequently encountered in the literature, namely the form of the virial theorem for bounded motions.

VIRIAL THEOREM. *Under the conditions of above, suppose $E \in \mathbb{R}$ such that the set $H^{-1}(E)$ is compact, then for each set of initial conditions $(q_0 p_0) \in \mathbb{R}^{2n}$ for which $H(q_0, p_0) = E$ one has*

$$2a\langle T\rangle_{q_0 p_0} = \left\langle \left.\frac{d(g^*(\lambda)H)}{d\lambda}\right|_{\lambda=0} \right\rangle_{q_0 p_0} \tag{13}$$

and if $g\star(\lambda)H = (\exp b\lambda)H$, *then*

$$2a\,\langle T\rangle_{q_0 p_0} = b\,E \tag{14}$$

where $\langle f\rangle_{q_0 p_0} = \lim_{T\to\infty} \frac{1}{T}\int_0^T \mathrm{d}t\, f_t(q_0, p_0)$ *for* $f \in A(\Gamma)$ *and* $f_t(q_0, p_0)$ *the solution of* (7).

Proof. The theorem follows from (11) and (12) and the boundedness of $\phi + \frac{a}{2}\sum_i p^i q^i$ on a compact set. ■

In the familiar applications of the virial theorem one mainly restricts oneself to the one-parameter groups of scale transformations (see e.g. [2]). In this case the function ϕ is a multiple of $\sum_i p^i q^i$. Wellknown examples are potentials which are homogeneous in the coordinates $q^k (k = 1, \ldots, n)$ e.g. the harmonic oscillator, the Kepler motion, a charged particle in an electromagnetic field with homogeneous vector potential, etc. We will not enter into the discussion of those wellknown examples.

Here we want to stress that the applicability of our theorem is not restricted to the scale transformations but opens a wide horizon of possibilities. As a simple but non-trivial illustration we discuss the Toda-lattice system where we combine a scale transformation of the p-coordinates with translations for the q-coordinates.

The Hamiltonian of the system in given by [10]

$$\begin{aligned} H(q,p) = \sum_{i=-n}^{n} (p^i)^2 + \sum_{i=-n}^{n-1} \left\{ \frac{\mathrm{d}}{b}\, e^{-b(q^{i+1}-q^i-\delta)} + \mathrm{d}(q^{i+1}-q^i) \right\} + \\ + P(q^n - q^{-n}) \end{aligned} \tag{15}$$

where $\delta, b, \mathrm{d}, P \in \mathbb{R}$ and $b\mathrm{d} > 0$.

One looks upon this system as a chain of $2n+1$ particles with anharmonic interaction with an equilibrium distance between the particles given by δ. By a simple transformation one eliminates δ; the coordinates q^i represent then the deviation from their equilibrium. As boundary condition a constant force of strength P is applied at the endpoints. The constant P has the meaning of a pressure.

Consider the one-parameter group of transformations $G = \{g(\lambda) \mid \lambda \in \mathbb{R}\}$ where

$$g(\lambda) q^k = q^k - k\lambda; \qquad g(\lambda) p^k = e^{b\lambda/2} p^k$$

$k = -n, -n+1, \ldots, n$. For all $\lambda \in \mathbb{R}$, $g(\lambda)$ is a canonical transformation with valence $c(\lambda) = \exp \frac{b\lambda}{2}$, and therefore $a = b/2$ in formula (2). We compute the function ϕ defined in formula (4) for X_1 as in (5):

$$\phi(q,p) = -\sum_{k=-n}^{n} \left(k\,p^k + \frac{b}{4}\, q^k p^k \right).$$

One checks that the Hamiltonian (15) transforms under G as follows:

$$g^*(\lambda)H(q,p) = e^{b\lambda} H(q,p) - (\mathrm{d} + P)(2n\,\lambda + e^{b\lambda}(q^n - q^{-n})).$$

Hence

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\, (g^*(\lambda)H(q,p))\Big|_{\lambda=0} = bH - (\mathrm{d} + P)(2n + b(q^n - q^{-n})). \tag{16}$$

Denote by

$$V(q) = \sum_{i=-n}^{n-1} \left(\frac{\mathrm{d}}{b}\, e^{-b(q^{i+1} - q^i)} + \mathrm{d}(q^{i+1} - q^i) \right)$$

the potential function and apply the virial theorem. One gets using (16):

$$\bar{r} = \frac{\langle \bar{V} \rangle_{q_0 p_0}}{\mathrm{d}} - \frac{\mathrm{d} + P}{\mathrm{d}b} \tag{17}$$

where $\bar{r} = \frac{\langle q^n - q^{-n} \rangle_{q_0 p_0}}{2n}$ is the mean distance between two neighbouring particles, and where

$$\langle \bar{V} \rangle_{q_0 p_0} = \frac{\langle V \rangle_{q_0 p_0}}{2n}$$

is the mean potential energy per particle. Remark that formula (17) is the expression for the time averages holding for all initial conditions $(q_0 p_0)$ and coinciding with the one calculated for thermal averages in [10].

One can also put the result (17) in the following form:

$$\bar{r} = \frac{E_0 - \langle \bar{T} \rangle_{q_0 p_0}}{\mathrm{d} + P} - \frac{1}{b}$$

where T is the kinetic energy and where $E_0 = H(q_0, p_0)/2n$. Using the ergodic theorem and the equipartition theorem

$$\langle \overline{T} \rangle_{q_0 p_0} = \frac{kT}{2}$$

one gets

$$\bar{r} = \frac{E_0 - kT/2}{\mathrm{d} + P} - \frac{1}{b} . \tag{18}$$

Take now the harmonic lattice with

$$H = \sum_i (p_i)^2 + \frac{\mathrm{d}b}{2} \sum_{i=-n}^{n-1} (q^{i+1} - q^i)^2 + P(q^n - q^{-n}) + \frac{\mathrm{d}}{b} 2n$$

and the dilation group

$$g(\lambda)p = e^{\lambda/2} p$$

$$g(\lambda)q = e^{\lambda/2} q .$$

Then

$$g^*(\lambda)H = e^{\lambda} H - (e^{\lambda} - e^{-\lambda/2}) P(q^n - q^{-n}) - (e^{\lambda} - 1) \frac{\mathrm{d}}{b} 2n$$

and applying formula (13) one gets as $a = b = 1$

$$2 \frac{\langle T \rangle_{q_0 p_0}}{2n} = \frac{\langle H \rangle_{q_0 p_0}}{2n} - \frac{1}{2} P\bar{r} - \frac{\mathrm{d}}{b} .$$

Again using the equipartition theorem:

$$E_0 = kT + \frac{1}{2} P\bar{r} + \frac{\mathrm{d}}{b} .$$

For small anharmonicity ($\mathrm{d} \gg 1$, $b \ll 1$, $\mathrm{d}b = \text{constant}$) this expression of the energy can serve as a first approximation in formula (18) and one gets:

$$\bar{r} = \frac{kT}{2\mathrm{d} + P} - \frac{2P}{b(2\mathrm{d} + P)} .$$

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