

VARIATIONAL PRINCIPLE AND PHASE SPACE MEASURE IN NON-CANONICAL COORDINATES

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ABSTRACT. Non-canonical equations of motion are derived from a variational principle written in symplectic form. The invariant measure of phase space and the covariant expression for the entropy are derived from non-canonical transformations of coordinates. This shows that the geometry of non-canonical phase space is non trivial even if dynamics has no compressibility.

1. Introduction

Theoretical formalisms very often use non-canonical equations of motion. For example, the equations for Eulerian variables, that describe ideal continuous media, are in general non-canonical [1]. Non-canonical phase space flows can be derived from Hamiltonian dynamics by means of non-canonical transformations of phase space coordinates (i.e. transformations with Jacobian not equal to one) while non-Hamiltonian dynamics cannot be derived using only transformations of phase space coordinates. However, non-canonical dynamics has a certain likeness with energy-conserving non-Hamiltonian dynamics [2] (this latter is commonly used in molecular dynamics simulations). For this reason, non-canonical systems can be used to improve our understanding of non-Hamiltonian systems with a conserved energy [2]. In the following, the comparison between non-Hamiltonian and non-canonical system will be exploited to clarify some issues regarding phase space measure. It will be shown that the invariant measure of non-canonical phase space can be derived from coordinate transformations without the need to consider dynamical properties, such as phase space compressibility. The situation is different in the non-Hamiltonian case, where one has to resort to arguments associated with time evolution in phase space [2, 3]. Coordinate transformations will be also used to obtain the covariant form of the entropy functional and a variational principle for non-canonical equations of motion, arising from a symplectic form of the action.

This paper is organized as follows: in Section 2 the action is written by means of the symplectic matrix and Hamiltonian equations in canonical form are derived from the variational principle. In Section 3 coordinate transformations will be applied to the symplectic form of the action in order to obtain non-canonical equations of motion from the variational procedure. In Section 4 it is shown how a certain class of non-Hamiltonian equations may be derived by introducing a coordinate-dependent scaling of time. Phase space invariant

measure and the covariant form of the entropy functional are obtained from coordinate transformations in Section 5. Finally, conclusions are given in Section 6.

2. Hamiltonian Canonical Equations in Symplectic Form

Consider a general time-independent Hamiltonian \mathcal{H} . Points in a $2N$ -dimensional phase space will be indicated by $x = (q, p)$. Consider also the symplectic matrix [4, 5]

$$(1) \quad \mathbf{B}^c = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix},$$

with the following properties

$$(2) \quad [\mathbf{B}^c]^T = -\mathbf{B}^c,$$

$$(3) \quad [\mathbf{B}^c]^{-1} = -\mathbf{B}^c.$$

Canonical Hamiltonian equation of motion are written in symplectic form [4, 5] as

$$(4) \quad \dot{x}_i = B_{ij}^c \frac{\partial \mathcal{H}}{\partial x_j}.$$

In the above equation and in the following ones, Einstein's convention of summing over repeated indices must be understood. The free indices assume all the values within their range of variation, which depends on the dimension of phase space. Usually, one first derives Hamiltonian equations and then shows that they can be written in symplectic form [4, 5]. It can be shown that Eq.s (4) can be obtained directly from the variational principle $\delta \mathcal{A} = \int dt [p\dot{q} - \mathcal{H}] = 0$, where \mathcal{A} is the action. To this end, one starts from the action

$$(5) \quad \mathcal{A} = \int dt [p\dot{q} - \mathcal{H}] = \int dt \left[\frac{1}{2} (p\dot{q} - q\dot{p}) - \mathcal{H} \right],$$

where the last equality is obtained by means of an integration by parts. Noticing that

$$(6) \quad p\dot{q} - q\dot{p} = \begin{bmatrix} \dot{q} & \dot{p} \end{bmatrix} \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} q \\ p \end{bmatrix},$$

the action can be expressed by means of the symplectic matrix \mathbf{B}^c as

$$(7) \quad \mathcal{A} = \int dt \left[\frac{1}{2} \dot{x}_i B_{ij}^c x_j - \mathcal{H} \right].$$

Applying the variational procedure one gets

$$(8) \quad \begin{aligned} \delta \mathcal{A} &= \int dt \left[\frac{1}{2} \delta \dot{x}_i B_{ij}^c x_j + \frac{1}{2} \dot{x}_i B_{ij}^c \delta x_j - \frac{\partial \mathcal{H}}{\partial x_j} \delta x_j \right] \\ &= \int dt \delta x_j \left[\dot{x}_i B_{ij}^c - \frac{\partial \mathcal{H}}{\partial x_j} \right] = 0. \end{aligned}$$

Finally, using $B_{ij}^c B_{jk}^c = \delta_{ik}$, the equations of motion (4) are obtained.

3. Non-canonical equations of motion

Consider a set of phase space coordinates $z = z(x)$ obtained using a transformation with Jacobian $\mathcal{J} = \left| \frac{\partial x}{\partial z} \right| \neq 1$. Such coordinates are non-canonical [1, 4, 5]. Under non-canonical transformations, the Hamiltonian transforms as a scalar according to $\mathcal{H}(x(z)) = \mathcal{H}'(z)$ and Eq.s (4) become:

$$(9) \quad \dot{z}_n = B_{nm} \frac{\partial \mathcal{H}'}{\partial z_m},$$

where the antisymmetric matrix

$$(10) \quad B_{nm} = \frac{\partial z_n}{\partial x_i} B_{ij}^c \frac{\partial z_m}{\partial x_j}$$

has been introduced. Equations (9) are referred as non-canonical Hamiltonian equations [1, 5]. They might introduce a compressibility in phase space

$$(11) \quad \kappa = \frac{\partial \dot{z}_n}{\partial z_n} = \frac{\partial B_{nm}}{\partial z_n} \frac{\partial \mathcal{H}'}{\partial z_m},$$

but one can also have non-canonical equations with zero compressibility [1]. In the following, it will be shown that Eq.s (9) can be derived from a variational principle. To this end, one applies a non-canonical transformation of coordinates to the symplectic expression of the action, Eq. (7):

$$(12) \quad \mathcal{A} = \int dt \left[\frac{1}{2} \frac{\partial x_i}{\partial z_m} \dot{z}_m B_{ij}^c x_j(z) - \mathcal{H}'(z) \right].$$

On the action expressed by Eq. (12) one can perform a variation on non-canonical coordinates and integrate by parts when needed. Thus, one obtains

$$(13) \quad \begin{aligned} \delta \mathcal{A} = & \int dt \left[\frac{1}{2} \frac{\partial^2 x_i}{\partial z_m \partial z_k} \delta z_k \dot{z}_m B_{ij}^c x_j(z) - \frac{1}{2} \frac{d}{dt} \left(\frac{\partial x_i}{\partial z_m} B_{ij}^c x_j(z) \right) \delta z_m \right. \\ & \left. + \frac{1}{2} \frac{\partial x_i}{\partial z_m} \dot{z}_m B_{ij}^c \frac{\partial x_j}{\partial z_k} \delta z_k - \frac{\partial \mathcal{H}'}{\partial z_k} \delta z_k \right]. \end{aligned}$$

Considering now the term

$$(14) \quad \begin{aligned} -\frac{1}{2} \frac{d}{dt} \left(\frac{\partial x_i}{\partial z_m} B_{ij}^c x_j(z) \right) \delta z_m &= -\frac{1}{2} \frac{d}{dt} \left(\frac{\partial x_i}{\partial z_k} B_{ij}^c x_j(z) \right) \delta z_k \\ &= -\frac{1}{2} \left(\frac{\partial^2 x_i}{\partial z_m \partial z_k} \dot{z}_m B_{ij}^c x_j(z) \right. \\ &\quad \left. + \frac{\partial x_i}{\partial z_k} B_{ij}^c \frac{\partial x_j}{\partial z_m} \dot{z}_m \right) \delta z_k, \end{aligned}$$

and substituting into Eq. (13) one finds

$$(15) \quad \delta \mathcal{A} = \int dt \delta z_k \left[\frac{\partial x_i}{\partial z_m} B_{ij}^c \frac{\partial x_j}{\partial z_k} \dot{z}_m - \frac{\partial \mathcal{H}'}{\partial z_k} \right],$$

which leads to equations in the form

$$(16) \quad \dot{z}_m \frac{\partial x_i}{\partial z_m} B_{ij}^c \frac{\partial x_j}{\partial z_k} = \frac{\partial \mathcal{H}'}{\partial z_k}.$$

By inverting the matrix

$$(17) \quad A_{mk} = \frac{\partial x_i}{\partial z_m} B_{ij}^c \frac{\partial x_j}{\partial z_k},$$

one finds the equations already given in (9) with B_{sk} given by Eq. (10). It is worth to remark that Eq.s (9) are still Hamiltonian although expressed in non-canonical form [1, 5]. As a matter of fact, a generalized bracket satisfying the Jacobi relation can be introduced [1, 2]. Considering the matrix B_{sk} defined in Eq. (10), the Jacobi relation leads to

$$(18) \quad B_{in} \frac{\partial B_{jk}}{\partial x_n} + B_{kn} \frac{\partial B_{ij}}{\partial x_n} + B_{jn} \frac{\partial B_{ki}}{\partial x_n} = 0.$$

4. Non-Hamiltonian equations of motion

Non-Hamiltonian equations of motion with a conserved energy [2] may be defined using the structure of Eq.s (9). To this end, one uses an antisymmetric matrix \mathbf{B}^{NH} which is no longer defined by Eq. (10) and does not satisfies the Jacobi relation as given by Eq. (18). Originally, Nosé [6] showed that a certain class of energy conserving non-Hamiltonian equations can be derived by combining non-canonical transformation of phase space coordinates and position-dependent scalings of time. Here it is shown how this can be achieved when starting from the variational principle in symplectic form. To this end, one considers the expression obtained by performing the variation of the action using non-canonical variables

$$(19) \quad \delta \mathcal{A} = \int dt \delta z_k \left(\dot{z}_m \frac{\partial x_i}{\partial z_m} B_{ij}^c \frac{\partial x_j}{\partial z_k} - \frac{\partial \mathcal{H}'}{\partial z_k} \right).$$

A position-dependent scaling of time is then applied

$$(20) \quad dt = \phi(z) d\tau.$$

In general, the above time scaling will depend on the path in phase space. Then one obtains

$$(21) \quad \dot{z}_s = B_{sk}^{NH} \frac{\partial \mathcal{H}'}{\partial z_k},$$

with

$$(22) \quad B_{sk}^{NH} = \phi^{-1}(z) \frac{\partial z_s}{\partial x_n} B_{nl}^c \frac{\partial z_k}{\partial x_l}.$$

Equations (21), are non-Hamiltonian since, in general, the Jacobi relation, Eq. (18), will not be satisfied because of the new matrix defined in Eq. (22). Phase space compressibility for Eq. (21) is defined as

$$(23) \quad \kappa^{NH} = -\phi^{-2}(z) \frac{\partial \phi}{\partial z_s} B_{sk} \frac{\partial \mathcal{H}'}{\partial z_k} + \phi^{-1}(z) \frac{\partial B_{sk}}{\partial z_s} \frac{\partial \mathcal{H}'}{\partial z_k}.$$

The first term on the right hand side is proportional to the time derivative of ϕ considering its evolution under the non-canonical flow (instead of the non-Hamiltonian one). The second term is proportional to the compressibility arising from the non-canonical transformation of coordinates. This two terms are combined with the scaling function ϕ to give the non-Hamiltonian compressibility κ^{NH} . If both terms are zero, the non-Hamiltonian flow will have zero compressibility.

5. Invariant Measure

Using canonical coordinates, averages in phase space are defined as [9]

$$(24) \quad \langle a \rangle = \int dx f(x) a(x),$$

where $f(x)$ is the normalized distribution function and a is an arbitrary phase space observable. Considering a transformation to non-canonical coordinates, one obtains

$$(25) \quad \int dx f(x) \rightarrow \int dz \left| \frac{\partial x}{\partial z} \right| f'(z) = \int dz \rho(z),$$

where the Jacobian $\mathcal{J} = \partial x / \partial z \neq 1$ is used to define the measure of non-canonical phase space. The Jacobian can be absorbed into a properly defined distribution function

$$(26) \quad \rho(z) = \left| \frac{\partial x}{\partial z} \right| f'(z),$$

which can be shown to obey a generalized Liouville equation [2]. As it will be shown in the following, this is particularly important when defining the entropy.

It is now easy to show that the measure in phase space, introduced by the change of coordinates, is also invariant in time. To this end, consider

$$(27) \quad dz(t) \left| \frac{\partial x(t)}{\partial z(t)} \right| = dz(0) \left| \frac{\partial z(t)}{\partial z(0)} \right| \left| \frac{\partial x(t)}{\partial x(0)} \right| \left| \frac{\partial x(0)}{\partial z(0)} \right| \left| \frac{\partial z(0)}{\partial z(t)} \right|.$$

By hypothesis $\left| \frac{\partial x(t)}{\partial x(0)} \right| = 1$ since x coordinates are canonical. Hence

$$(28) \quad dz(t) \left| \frac{\partial x(t)}{\partial z(t)} \right| = dz(0) \left| \frac{\partial z(t)}{\partial z(0)} \right| \left| \frac{\partial x(0)}{\partial z(0)} \right| \left| \frac{\partial z(0)}{\partial z(t)} \right|.$$

Noticing that $\left| \frac{\partial z(t)}{\partial z(0)} \right| \left| \frac{\partial z(0)}{\partial z(t)} \right| = 1$, one gets the result

$$(29) \quad dz(t) \left| \frac{\partial x(t)}{\partial z(t)} \right| = dz(0) \left| \frac{\partial x(0)}{\partial z(0)} \right|.$$

Equation (29) shows that the Jacobian of the non-canonical transformation of coordinates automatically provides the invariant measure in phase space. It is worth to remark that no special property of the dynamics was used in the derivation and, in particular, no mention has been made of phase space compressibility.

Tuckerman et al [3] defined an invariant measure for systems with a non-zero compressibility in phase space. Such systems may be either non-canonical or non-Hamiltonian. In order to arrive at the definition of the invariant measure, they considered a Jacobian associated to phase space flow

$$(30) \quad \mathcal{J}_t(t, t_0) = \left| \frac{\partial z(t)}{\partial z(t_0)} \right|.$$

This Jacobian obeys the equation of motion

$$(31) \quad \frac{d}{dt} \mathcal{J}_t = \kappa \mathcal{J}_t ,$$

which can be integrated to yield

$$(32) \quad \begin{aligned} \mathcal{J}_t(t, t_0) &= e^{\int_{t_0}^t \kappa(t') dt'} = e^{w(t) - w(t_0)} \\ &= e^{w(t)} e^{-w(t_0)} , \end{aligned}$$

where w is the primitive function of the compressibility κ . Then the invariant measure can be defined as [3]

$$(33) \quad dz(t) e^{-w(t)} = dz(t_0) e^{-w(t_0)} .$$

For non-canonical systems with compressibility

$$(34) \quad \mathcal{J}_t(t, t_0) = \left| \frac{\partial z(t)}{\partial x(t)} \right| \left| \frac{\partial x(t_0)}{\partial z(t_0)} \right| ,$$

where it has been used $|\partial x(t)/\partial x(t_0)| = 1$, which is true since the x coordinates are canonical by hypothesis. In this case, one is led to the identification

$$(35) \quad e^{w(t)} = \left| \frac{\partial z(t)}{\partial x(t)} \right| ,$$

$$(36) \quad e^{-w(t_0)} = \left| \frac{\partial x(t_0)}{\partial z(t_0)} \right| ,$$

so that the invariant measure proposed by Tuckerman et al, Eq. (33), and that given in Eq. (29) agrees. However, if a particular non-canonical system ($\mathcal{J} \neq 1$) has no compressibility, one finds $\mathcal{J}_t = 1$ so that the invariant measure given in Eq. (33) cannot be used. Instead, the invariant measure given in Eq. (29) is still correct.

Proper consideration of the invariant measure is critical when defining the entropy functional [3, 7, 8]. For a Hamiltonian system, Gibb's entropy S is given by [9]

$$(37) \quad S = -k_B \int dx f(x) \ln f(x) .$$

Performing a non-canonical transformation of variables one must take into account the Jacobian so that in the new coordinates the entropy is given by:

$$(38) \quad S = -k_B \int dz \rho(z) \ln f'(z) ,$$

where $\rho(z)$ is defined in Eq. (26). If the non-canonical system has a non-zero compressibility $\rho(z) = e^{-w} f'(z)$ and Eq. (38) would be equal to that proposed by Tuckerman. When the compressibility is zero Tuckerman's approach cannot be used because one would find incorrectly a trivial phase measure. Instead, Equation (38), with $\rho(z)$ defined in Eq. (26), can be used rigorously in order to describe non-canonical systems of all types, with or without phase space compressibility.

This analysis suggests that analogous considerations apply in the case of non-Hamiltonian systems: when a non-Hamiltonian system has zero compressibility Tuckerman's recipe

would give incorrectly a trivial measure. Therefore, it is clear that a more rigorous formulation of non-Hamiltonian statistical mechanics is needed.

6. Conclusions

A formalism for Hamiltonian systems in non-canonical coordinates has been presented. Non-canonical equations of motion have been derived directly from a variational principle written in symplectic form. It has been shown how a certain class of non-Hamiltonian equations of motion may be derived by means of coordinate-dependent scalings of time. Finally, the invariant measure of phase space and the covariant definition of the entropy functional have been obtained from the Jacobian of non-canonical transformations of coordinates. There may be cases where the dynamical compressibility is zero. In these cases, Tuckerman's recipe would give an incorrect phase space measure because non-canonical coordinates have in general a non-trivial Jacobian that must be considered in order to define the invariant measure. The formalism here presented naturally takes this into account. The results here derived for non-canonical Hamiltonian systems have also implications for non-Hamiltonian statistical mechanics. As a matter of fact, there are non-Hamiltonian systems with zero phase space compressibility. Again, in these cases Tuckerman's approach would give an incorrect measure. In conclusion, a rigorous non-Hamiltonian statistical mechanics is still to be found. This problem will be addressed in future papers.

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