University of Groningen

Passivity and equilibrium for classical Hamiltonian systems

Daniels, HAM

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version
Publisher's PDF, also known as Version of record

[Link to publication in University of Groningen/UMCG research database](#)

Passivity and equilibrium for classical Hamiltonian systems

H. A. M. Daniëls

Passivity and equilibrium for classical Hamiltonian systems

H. A. M. Daniëls

Instituut voor Theoretische Natuurkunde, Rijksuniversiteit Groningen Postbus 800, Groningen, The Netherlands

For classical continuous n-particle systems equilibrium states are characterized by a condition of passivity.

INTRODUCTION

In statistical mechanics one describes the equilibrium states by a density function (operator) of the form $\rho = e^{-\beta H}/Z$. The aim of this paper is to give for classical systems a justification for this from the second law of thermodynamics: If a system is in equilibrium, no work is performed by the system if the external parameters are varied in a certain (cyclic) way.

The notion of passivity has been introduced in Ref. 1 and the equivalence of equilibrium, KMS, and complete passivity established for abstract C^*-dynamical systems, where, as in fermion and lattice systems, the dynamics is given by a strongly continuous one-parameter group of automorphisms. In a related paper[2] the notion of passivity is discussed, for finite quantum spin systems, in detail. This problem has not been treated yet for continuous classical systems. Therefore we will consider here classical continuous systems consisting of n-point masses, and realize a program analogous to the one in Ref. 2.

The main part of this paper deals with the characterization of passive states by a very simple condition on the density function (Theorem 1). The rest of the results follow from this Theorem and investigations similar to those given in Ref. 2. As far as we know, the proof of Theorem 1 is essentially new. In Ref. 1 part of the results is proved relying on the algebraic structure for KMS states as obtained in Ref. 3, whereas in this paper we rather use symplectic geometry.

1. NOTATION AND DEFINITIONS

In this section we fix the notation and quote some standard results on Hamiltonian mechanics; for more details see, e.g., Refs. 4–6.

A n-particle classical system S is described by (M^{2k}, Ω, H), where M^{2k} is a symplectic manifold (the cotangent bundle of the configuration manifold), Ω the canonical symplectic 2-form, and H the Hamilton function on M^{2k}. [One could think of $M^{2k} = (\mathbb{R}^d \times \mathbb{R}^d)^n$ if the particles move freely in d-dimensional Euclidean space or $M^{2k} = (T^d \times \mathbb{R}^d)^n$ if the particles are enclosed in a box with periodic boundary conditions.] In the following we write M for M^{2k}. λ will denote the Liouville measure on M. Let us introduce some function spaces on M.

$C^\infty(M)$ is the set of (real) C^∞-functions on M.

$C_0^\infty(M)$ is the subset of functions with compact support.

$C^0(M)$ is the set of (complex) continuous functions which have a limit at infinity.

$L^2(M, \lambda)$ is the set of (complex) L^2-functions with respect to λ. $\mathfrak{A}$ is the C^*-algebra of (complex) continuous functions on $\bar{M}$, where $\bar{M}$ is the one point compactification of M. As a set, $\mathfrak{A}$ equals $C^0(M)$.

The Poisson bracket is a bilinear map $\{\ ,\ \}:C_0^\infty(M) \times C_0^\infty(M) \mapsto C_0^\infty(M)$ such that for all f, g, $h \in C_0^\infty(M)$:

(p1) Skew-symmetry: $\{f, g\} = -\{g, f\}$;

(p2) Jacobi identity:
$\{\{f, g\}, h\} + \{\{h, f\}, g\} + \{\{g, h\}, f\} = 0$;

(p3) Leibnitz rule: $\{fg, h\} = \{f, h\} \cdot g + \{g, h\} \cdot f$.

λ diff(M), resp. S diff(M), is the set of λ-(volume)-preserving, resp. symplectic (Ω-preserving), diffeomorphisms on M. λ diff$_0(M)$ and S diff$_0(M)$ are the subsets consisting of diffeomorphisms which differ from the identity only in a compact subset of M. S diff$_0(M) \sim$ id will denote the C^∞-connected component of the identity in S diff$_0(M)$. The following are in one-to-one correspondence:

$H \in C^\infty(M)$ locally defined;

X_H local Hamiltonian vector field with Hamilton function H;

$L_H:C^\infty(M) \mapsto C^\infty(M)$ the Liouville operator defined by $L_H(f) = \{f, H\}$;

$(\phi_t)_{t \in \mathbb{R}}$ the phase flow, a one-parameter group in S diff(M) defined for small $|t|$.

The correspondence is defined by the following formulas:

$$\frac{d}{dt}\bigg|_{t=0} \phi_t(x) = X_H(x),$$

$$\frac{d}{dt}\bigg|_{t=0} f(\phi_t(x)) = (L_H f)(x) = \{f, H\}(x).$$

Given a Hamilton function H, the equations of motion in local coordinates read:

$$\dot{p}_i = -\frac{\partial H}{\partial q_i}, \quad p_i(0) = p_{i0},$$

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad q_i(0) = q_{i0}.$$

Write $(p, q) = x$. The solution of these equations $x_t = \phi_t(x_0)$ defines the phase flow ϕ_t. If the Hamiltonian is time-dependent, we write $x_t = \phi_{t,s}(x_s)$, where $\phi_{t,s}$ is the flow from s to t along the trajectories of the solutions of the equations of motion with initial condition $x(s) = x_s$. $\phi_{t,s}$ is no longer a one-parameter group, but one has $\phi_{t,s} = \phi_{t,u} \circ \phi_{u,s}$. If $\phi \in \lambda$ diff(M), a unitary linear operator $\phi^*: L^2(M, \lambda) \to L^2(M, \lambda)$ is defined by transposition:

$$\phi^*(f) = f \circ \phi.$$

0022-2488/81/040843-04$1.00

A state ω of the system S is a normalized positive linear functional on $\mathfrak{A}$:

$$\omega(f) = \int_M f\, d\mu,$$

where μ is a normalized, regular, Borel measure on M. We only consider states which are given by a positive density function ρ:

$$\frac{d\mu}{d\lambda} = \rho \in L^1(M, \lambda).$$

Perturbations of the dynamics: We assume that the field X_H is full and therefore the corresponding phase flow ϕ_t is defined for all $t \in \mathbb{R}$. This guarantees that all differential equations considered in the sequel have solutions defined for all $t \in \mathbb{R}$.

Definition 1: A perturbation is a family $(h_t)_{t \in \mathbb{R}}$ in $C_0^\infty(M)$ such that:

(h1) $(t,x) \mapsto h_t(x)$ is smooth;

(h2) $h_t = 0$ for $t \notin (0,T)$;

(h3) $\bigcup_{t \in \mathbb{R}} \mathrm{supp}(h_t)$ is contained in a compact subset of M.

The perturbed phase flow corresponding to the time-dependent Hamiltonian $H + h_t$ is denoted by $\psi_{t,s}$.

2. PASSIVITY, COMPLETE PASSIVITY, AND STATEMENT OF THE RESULTS

Given the perturbation h_t, we define (cf. Ref. 1)

$$l^h := \int_0^T \psi_{t,0}^* \left(\frac{dh_t}{dt}\right) dt \in \mathfrak{A}.$$

Definition 2: ω is called a passive state if for all perturbations h_t, $\omega(l^h) \geqslant 0$.

Theorem 1: ω is passive if and only if ρ is decreasing with respect to H, i.e., for all $x, y \in M$

$$H(x) > H(y) \Rightarrow \rho(x) \leqslant \rho(y). \tag{1}$$

Corollary: A Gibbs state is passive.

For every $m \in \mathbb{N}$ we consider the system $S^m = (M^m, \Omega^m, H^m)$, where

$$M^m = \underbrace{M \times M \times \cdots \times M}_{m \text{ times}},$$

$$\Omega^m = \overset{m}{\oplus} \Omega,$$

$$H^m = H \otimes 1 \otimes \cdots \otimes 1 + \cdots + 1 \otimes \cdots \otimes 1 \otimes H.$$

If ω is a state on $\mathfrak{A}$ with density ρ, then $\omega^{\otimes m}$ is the state on $\mathfrak{A}^{\otimes m}$ with density function ρ^m defined by

$$\omega^{\otimes m}(f_1 \otimes \cdots \otimes f_m) = \omega(f_1) \cdot \omega(f_2) \cdots \omega(f_m),$$

$$\rho^m(x_1, x_2, \ldots, x_m) = \rho(x_1) \cdots \rho(x_m).$$

Definition 3: ω is completely passive if $\omega^{\otimes m}$ is passive state for the system S^m for all $m \in \mathbb{N}$.

Theorem 2: ω is completely passive if and only if $\rho = e^{-\beta H}/Z$ with $0 \leqslant \beta \leqslant \infty$.

3. PROOFS OF THEOREMS 1 AND 2

Let us first compute $\omega(l^h)$. We start with a perturbation h_t of the Hamiltonian H. Let ϕ_t respectively $\psi_{t,s}$ denote the phase flows corresponding to H respectively $H + h_t$. Then by partial integration (cf. Ref. 1)

$$l^h = -\int_0^T \left(\frac{d}{dt} \psi_{t,0}^*\right) h_t\, dt. \tag{1a}$$

Define

$$\gamma_t = \phi_{-t} \psi_{t,0} \tag{2}$$

so that

$$\gamma_t^* = \psi_{t,0}^* \, \phi_{-t}^*.$$

Bearing in mind the formulas

$$\frac{d}{dt} \phi_t^* = \phi_t^* L_H,$$

$$\frac{d}{dt} \psi_{t,0}^* = \psi_{t,0}^* L_{H + h_t},$$

$$\phi^*\{f, g\} = \{\phi^* f, \phi^* g\} \quad \text{for symplectic } \phi,$$

we find

$$\begin{aligned}
\frac{d}{dt} \gamma_t^* &= \frac{d}{dt} (\psi_{t,0}^* \, \phi_{-t}^*) \\
&= \psi_{t,0}^* L_{H + h_t} \phi_{-t}^* - \psi_{t,0}^* \phi_{-t}^* L_H \\
&= \gamma_t^* \phi_t^* (L_{H + h_t} - L_H) \phi_{-t}^* \\
&= \gamma_t^* L_{\phi_t^* h_t}.
\end{aligned} \tag{3}$$

On the other hand,

$$\begin{aligned}
\left(\frac{d}{dt} \psi_{t,0}^*\right) h_t &= \psi_{t,0}^* L_H(h_t) = \gamma_t^* \phi_t^* L_H(h_t) \\
&= \gamma_t^* L_H(\phi_t^* h_t) = -\gamma_t^* L_{\phi_t^* h_t}(H)
\end{aligned}$$

and therefore

$$\left(\frac{d}{dt} \psi_{t,0}^*\right) h_t = -\frac{d}{dt} \gamma_t^*(H).$$

Hence $l^h = \gamma_T^*(H) - H$ and therefore ω is passive iff for all perturbations h_t

$$\omega(\gamma_T^*(H) - H) \geqslant 0. \tag{4}$$

We now characterize the set of γ_T's which can be obtained from a perturbation h_t. From (2) it is clear that $\gamma_T \in S$ diff(M), (3) and (h3) imply $\gamma_T \in S$ diff$_0(M)$. Since $\gamma_0 = \mathrm{id}$ and γ_t satisfies (3), $\gamma_T \in S$ diff$_0(M) \sim \mathrm{id}$. A very large class $\mathscr{E}$ of γ_T's is obtained by choosing h_t suitable. Take $T = 1$ and let $p \in \mathbb{N}$. Let $\alpha_j \in C^\infty([0,1] \to \mathbb{R})$ such that $\mathrm{supp}(\alpha_j') \subset [(j-1)/p, j/p]$, $\alpha_j((j-1)/p) = 0$ and $\alpha_j(j/p) = 1$, $j = 1, 2, \ldots, p$. Let $g_j \in C_0^\infty(M)$ arbitrary, $j = 1, \ldots, p$. Define

$$h_t = \sum_{j=1}^p \alpha_j'(t) \phi_{-t}^*(g_j).$$

Now (3) reads

$$\frac{d}{dt} \gamma_t^* = \gamma_t^* \alpha_j'(t) L_{g_j} \quad \text{for } \frac{j-1}{p} \leqslant t \leqslant \frac{j}{p}.$$

This equation can easily be solved, yielding

$$\gamma_1 = \exp(X_{g_p}) \circ \cdots \circ \exp(X_{g_1}) \tag{5}$$

and

$$\gamma_1^* = \exp(L_{g_1}) \circ \cdots \circ \exp(L_{g_p}) \,,$$

where $\exp(X_g)$ denotes the time 1 map corresponding to the Hamiltonian vector field X_g with Hamilton function g. Let $\mathscr{S}$ denote the set of γ's defined by (5). It follows from Ref. 7 that if $H^1(M,\mathbb{R}) = 0$, the class $\mathscr{S}$ coincides with S diff$_0(M)$-$\sim$id. So, if $H^1(M,\mathbb{R}) = 0$ [e.g., $M = (\mathbb{R}^d \times \mathbb{R}^d)^n$], one has:

Lemma 1: ω is passive iff (4) holds for all $\gamma \in S$ diff$_0(M)$-$\sim$id.

Lemma 2: A passive state is invariant.

Proof: Take $\gamma_t = \exp(tX_g)$, then (4) implies

$$\frac{d}{dt}\Big|_{t=0} \omega(\gamma_t^*(H) - H) = 0 \,.$$

Hence

$$\omega(\{\,g, H\,\}) = 0 \quad \text{for all } g \in C_0^\infty(M),$$

yielding the invariance of ω.

Remark: Using the classical KMS condition one shows easily that (4) holds for small $|t|$ if ω is a KMS state.[8] The problem is to show that (4) holds for all t.

Proof of Theorem 1: For the sake of simplicity we restrict ourselves to the case where $M = (\mathbb{R}^d \times \mathbb{R}^d)^n$ and ρ continuous. (This proof can be generalized easily for $\rho \in L^1$.[9])

Suppose ρ satisfies (1). To prove passivity, we prove, in view of Lemma 1, the *a priori* stronger assertion $\omega(\gamma^*(H) - H) \geqslant 0$ for all $\gamma \in \lambda$ diff$_0(M)$. Suppose there exists $\gamma \in \lambda$ diff$_0(M)$ such that

$$\int_M [H(x) - H(\gamma(x))]\, d\mu(x) = \epsilon > 0 \,.$$

This will lead to a contradiction. Let K be a cube in M such that $\gamma = $ id on K^c. Define

$$A: = \sup_{\substack{x,\, y \in K \\ x \neq y}} \frac{\|\gamma^{-1}(x) - \gamma^{-1}(y)\|}{\|x - y\|}$$

and

$$B: = \max_{x \in K} |H(x)|$$

$\|\ \|$ is just the Euclidean norm on $(\mathbb{R}^d \times \mathbb{R}^d)^n$. Since ρ is uniformly continuous on the cube K, there exists $\eta > 0$ such that for all $x, y \in K$

$$\|x - y\| < \eta \Rightarrow |\rho(x) - \rho(y)| < \frac{\epsilon}{8B \cdot \lambda(K)} \,.$$

Divide the cube K into N small cubic cells $C_1, C_2, \ldots, C_N$ of equal λ-measure: $\lambda(C_i) = \lambda(K)/N$ and diam(C_i)-$= [\lambda(K)/N]^{1/r} \cdot \sqrt{r}$, where $r = 2\,dn$. Choose N large enough to ensure

$$\left| \int_K H(x)\, d\mu(x) - \sum_{i=1}^N H(x_i)\mu(C_i) \right| \leqslant \frac{\epsilon}{8}, \tag{6}$$

$$\left| \int_K H(\gamma(x))\, d\mu(x) - \sum_{i=1}^N H(x_i)\mu(\gamma^{-1}(C_i)) \right| \leqslant \frac{\epsilon}{8}, \tag{7}$$

$$(A + 1)\left(\frac{\lambda(K)}{N}\right)^{1/r} \cdot \sqrt{r} \leqslant \eta \tag{8}$$

for all possible choices of $x_1, \ldots, x_N$ with $x_i \in C_i$. Using the

mean value theorem, we can choose $x_i \in \text{int}(C_i)$ such that

$$\mu(C_i) = \int_{C_i} \rho(x)\, d\lambda = \rho(x_i)\,\lambda(C_i), \quad i = 1, \ldots, N,$$

and then for all i and j

$$H(x_i) > H(x_j) \Rightarrow \mu(C_i) \leqslant \mu(C_j) \,. \tag{9}$$

We claim that there exists a permutation Π of $\{1,2,\ldots,N\}$ such that

$$C_{\Pi(i)} \cap \gamma^{-1}(C_i) \neq \emptyset, \quad i = 1,2,\ldots,N.$$

Indeed this follows from a theorem of Hall.[10] The Hall condition is fulfilled because γ^{-1} is λ-(volume)-preserving. Define $U_i = C_{\Pi(i)} \cup \gamma^{-1}(C_i)$; then, using (8),

$$\text{diam}(U_i) \leqslant (A + 1)\,\text{diam}(C_i) \leqslant \eta$$

and therefore

$$\begin{aligned}
|\mu(\gamma^{-1}(C_i)) &- \mu(C_{\Pi(i)})| \\
&= \left| \int_{\gamma^{-1}(C_i)} \rho(x)\, d\lambda - \int_{C_{\Pi(i)}} \rho(x)\, d\lambda \right| \\
&\leqslant \sup_{x,\, y \in U_i} |\rho(x) - \rho(y)| \cdot \lambda(U_i) \\
&\leqslant \frac{\epsilon}{8B\lambda(K)} \cdot 2\lambda(C_i) = \frac{\epsilon}{4BN} \,.
\end{aligned}$$

Hence

$$\left| \sum_{i=1}^N H(x_i)\mu(\gamma^{-1}(C_i)) - \sum_{i=1}^N H(x_i)\mu(C_{\Pi(i)}) \right| \leqslant \frac{\epsilon}{4} \,. \tag{10}$$

Combining (6), (7), and (10), we obtain

$$\sum_{i=1}^N H(x_i)\mu(C_i) - \sum_{i=1}^N H(x_i)\mu(C_{\Pi(i)}) \geqslant \frac{\epsilon}{2} > 0 \,.$$

This contradicts (9) (cf. Refs. 11 and 2).

Conversely, let ω be passive and suppose ρ does not satisfy (1). Then there exist $x, y \in M$ such that

$$H(x) > H(y) \quad \text{and} \quad \rho(x) > \rho(y) \,. \tag{11}$$

Since both H and ρ are continuous, there are small cells $C_1 \ni x$, $C_2 \ni y$ such that (11) holds on the cells. We now construct $\gamma \in \lambda$ diff$_0(M)$ which interchanges the cells C_1 and C_2 and $\lambda(\{x \in M \mid \gamma(x) \neq x \text{ and } x \notin C_1 \cup C_2\})$ is very small. If $M = \mathbb{R}^2$, one takes $\gamma = \exp X_g$, where X_g is the vector field of Fig. 1. The field goes to zero in the shaded area. In the higher dimensional case one proceeds as follows. Take a 2-dim sym-
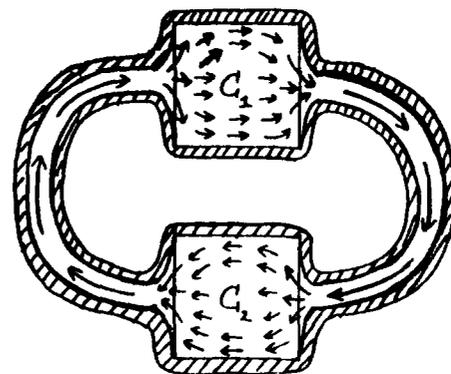

FIG. 1.

plectic plane P through x and y on which the symplectic 2-form is nondegenerate. Then take C_1 and C_2 to be two symplectomorphic cylindric cells symplectic-orthogonal to the 2-dim plane P. Take γ restricted to P the transformation of Fig. 1 and then extend to the symplectic orthogonal complement of the plane P. Following this method, one can construct γ with

$$\omega(\gamma^*(H) - H) < 0,$$

which contradicts the passivity of ω. □

Proof of Theorem 2: In view of Theorem 1 complete passivity is equivalent to the condition

$$H(x_1) + \cdots + H(x_m) > H(y_1) + \cdots + H(y_m)$$
$$\Rightarrow \rho(x_1) \cdots \rho(x_m) \leqslant \rho(y_1) \cdots \rho(y_m)$$

for all $(x_1,...,x_m) \in M^{\,m}$ and $(y_1,...,y_m) \in M^{\,m}$. The rest of the proof runs like the proof of Theorem 7 in Ref. 2. □

Remark: The "only if" part of Theorem 2 can also be proved using the techniques of Ref. 8.

Note added in proof: After this paper was submitted we received a preprint by J. Górecki and W. Pusz containing similar results obtained by different methods.

ACKNOWLEDGMENTS

I am indebted to H. Maassen and F. Takens for useful

discussions and to M. Winnink for asking the relevant questions and a critical reading of the manuscript.

[1] W. Pusz and S. L. Woronowicz, "Passive States and KMS states for General Quantum Systems," Commun. Math. Phys. **58**, 273–90 (1978).

[2] A. Lenard, "Thermodynamical Proof of the Gibbs Formula for Elementary Quantum Systems," J. Stat. Phys. **19**, 575–86 (1978).

[3] R. Haag, N. M. Hugenholtz, and M. Winnink, Commun. Math. Phys. **5**, 215 (1967).

[4] V. I. Arnold, *Mathematical Methods of Classical Mechanics*, Gretu Texts in Mathematics Vol. **60** (Springer, New York-Heidelbeg-Berlin, 1978).

[5] W. Thirring, *Lehrbuch der Mathematischen Physik* (Springer, New York-Vienna, 1977).

[6] A. M. Vinogradov and B. A. Kupershmidt, "The Structures of Hamiltonian Mechanics," Russian Math. Surv. **32**, 177–243 (1977).

[7] A. Banyaga, "Sur la structure du groupe des difféormorphismes qui préservent une forme symplectique," Comment Math. Helv. **53**, 174–227 (1978).

[8] B. Demoen, P. Vanheuverzwijn, and A. Verbeure, "Energetically stable systems," J. Math. Phys. **19** 2256–9 (1978).

[9] After we finished the manuscript M. Aizenman showed us a proof of the "if" part of the theorem for ρ, $H \in L^2(X, \mu)$ (X measure space), using integral representations for measurable functions.

[10] M. Hall, Jr., *Combinatorial Theory* (Blaisdell, Waltham, Mass., 1967), Theorem 5.1.1.

[11] G. H. Hardy, J. E. Littlewood, and G. Polya, *Inequalities* (Cambridge U. P.,Cambridge, 1934), Theorem 368.

846   J. Math. Phys., Vol. 22, No. 4, April 1981

H. A. M. Daniëls   846