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Classical mechanics in infinite-dimensional Hilbert space

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THE MECHANICS of a denumerably infinite set of particles constitutes in a sense an intermediate case between the usual mechanics of many-point systems and the continuum theory. In this paper we present some of the fundamental principles of classical mechanics in a real separable Hilbert space. Both kinematics and dynamics are investigated.

Mechanika nieskończonego przeliczalnego zbioru cząstek stanowi w pewnym sensie przypadek pośredni pomiędzy zwykłą mechaniką układu złożonego ze skończonej liczby cząstek a mechaniką ośrodków ciągłych. W pracy tej przedstawiono odpowiedniki postawowych pojęć i praw mechaniki klasycznej w nieskończenie wymiarowej rzeczywistej przestrzeni Hilberta. Rozpatrzono zarówno kinematykę jak i dynamikę układów o nieskończenie przeliczalnej liczbie stopni swobody.

Механика бесконечно счетного множества частиц составляет в некотором смысле промежуточный случай между обыкновенной механикой системы, состоящей из конечного количества частиц, и механикой сплошных сред. В настоящей работе представлены аналоги основных понятий и законов классической механики в бесконечномерном действительном гильбертовом пространстве. Рассмотрены так кинематика, как и динамика систем с бесконечным счетным количеством степеней свободы.

Introduction

THERE ARE many physical systems which have to be considered as systems with an infinite countable number of degrees of freedom. The most natural class of such systems which recently have been intensively studied is a system of infinitely many point particles. The fundamental problem arising when studying dynamical properties of such systems is: what is the set of initial conditions for which there exists a solution of the following infinite system of equations:

$$(*)\qquad \dot{q}_i = p_i, \quad \dot{p}_i = -\sum_{j\neq i}^{\infty} \mathrm{grad}\Phi(|q_i - q_j|), \quad i = 1, 2, \ldots,$$

where q_i, p_i, $i = 1, 2, \ldots$ denote respectively the position and momentum of the i-th point and Φ is an interaction potential.

This highly nontrivial problem was studied by LANFORD [8, 9] for classical point-particle systems interacting by means of a two-body bounded, smooth and short-range potential Φ. He proved an existence and uniqueness theorem for the system of equations (*) in the one-dimensional case, assuming that the initial density of positions $(q_i)_{i=1}^{\infty}$ is small enough and the initial momenta $(p_i)_{i=1}^{\infty}$ increase with the distance from the origin at most logarithmicaly i.e., $|p_i| < K \log_+ |q_i|$. In an unpublished paper Gnibre proved the existence and uniqueness theorem for the system of equations (*) in the three-dimensional case but with stronger restrictions on the initial data, namely he assumed that both density of momentum and density of position are bounded.

The result of Lanford was expanded some years later by DOBRUSHIN and FRITZ in two directions: allowing singular potentials [3], and two-dimensional systems [4]. Still later FRITZ improved this result [5] proving the existence of the dynamics for superstable interactions [5] of finite range in dimensions one and two; the above method, however, cannot be applied to a dimension greater than two.

Another approach to this problem was given by SINAI [13]. His method based on some probabilistic considerations connected with a GIBBS state μ [13], can be applied in any numbers of dimensions. Using this method, he was able to prove the existence theorem for the set of initial conditions which has measure μ equal to 1; this set, however, is not known explicitly.

Still another approach to this problems was presented by C. MARCHIORO *et al.* [11]. They considered the following Cauchy problem which is related to the dynamical problem (*):

$$\frac{d}{dt} f_t = \mathscr{L} f_t,$$

$$f_{t=0} = f, \quad f \in L_2(\mathscr{X}, \mu),$$

where

$$\mathscr{L} f = \sum_{i=1}^{\infty} \left\{ \frac{\partial f}{\partial q_i} p_i + \frac{\partial f}{\partial p_i} F_i(q) \right\} \quad \text{is the Liouville operator,}$$

$\mathscr{X}$ is phase space of the system (*), μ is Gibbs measure invariant with respect to the dynamics given by (*) and f is an element of algebra $\mathscr{U} \subset L_2(\mathscr{X}, \mu)$ called "observable". Each function in $\mathscr{U}$ depends only on the coordinates of particles that fall in the fixed bounded region. It is possible to show [6] that if $\mathscr{L}$ is essentialy antiself-adjoint on $\mathscr{U}$, there exists a dynamical flow $(\mathscr{X}, T_t, \mu)$ such that

$$(U_t f)(x) = f(T_t x), \quad t \in R, \quad x \in \mathscr{X}, \quad f \in L_2(\mathscr{X}, \mu),$$

where $U_t = e^{\bar{\mathscr{L}} t}$.

Marchioro et al. proved antiself-adjointness of the Liouville operator for a one-dimensional hard core system with singular two-body interaction. We see that in this approach the main idea is to study the time evolution of the functions describing microscopic state observables rather than the motion itself. Furthermore it was proved in [15] that by appropriate assumptions on the initial state μ, the phase space of a physical system can be reduced to the infinite-dimensional separable Hilbert space.

Other examples of systems with an infinite countable number of degrees of freedom appear when the required physical quantity related to the described phenomenon is a function $f(x, t)$ from Hilbert space $L_2(\Omega)$. The evolution operator in this case is usually some differential or integral operator (Schrödinger equation, Boltzmann equation) acting on the space $L_2(\Omega)$. The function $f(x, t)$ can be expanded into Fourier series in an orthonormal complete basis $e_i(x) \in L^2(\Omega)$, $i = 1, 2, \ldots$.

$$f(x, t) = \sum_{i=1}^{\infty} q_i(t) e_i(x).$$

It is easy to see that the time evolution of the function $f(x, t)$ is equivalent to the time evolution of its Fourier coefficients $(q_i(t))_{i=1}^{\infty}$. The phase space here is also the Hilbert space: namely the space l^2.

The above considerations and the fact that the infinite set of particles constitutes, in a sense, an intermediate case between the usual mechanics of many-point systems and the continuum theory, prove the necessity of constructing a direct counterpart of classical mechanics [1, 14] in infinite-dimensional separable Hilbert space. The present paper is devoted to this problem.

One of the most interesting transitions from the finite-dimensional to the infinite-dimensional mechanics have been given by LAX [10]. He defined the counterparts of the basic concepts of classical mechanics in the infinite-dimensional case and put the Korteweg–de Vries equation in Hamilton formalism. Thus he proved the existence of an infinite system of conserved functionals for this equation. In our paper, we do not postulate Hamilton equations but derive these equation from the variational principle. In addition we give the definition and the fundamental properties of the divergence of velocity. This concept of divergence plays an important role in the derivation of the infinite-dimensional counterpart of the Liouville equation [15, 16].

1. The kinematics of motion

1.1. The mapping $X \to x$

Consider a homeomorphism $f: X \to x$, $X, x \in H$, of a real separable Hilbert space onto itself; the inverse mapping will be denoted by $g: x \to X$. Assume that f is continuously Fréchet differentiable, i.e., the mapping $X \to Df(X)$ is continuous and the linear operator $Df(X)$ is a linear homeomorphism of H onto itself. Then the Fréchet derivative $Dg(x)$ is also continuous and the linear operator $Dg(x)$ is a linear homeomorphism inverse to $Df(X)$.

$$Df(X) \circ Dg(x) = Dg(x) \circ Df(X) = I. \tag{1.1}$$

Frequently, if no confusion results, we shall write $x(X)$ rather than $f(X)$ and $X(x)$ instead of $g(x)$.

We shall also consider the mapping $f:(X, t) \to x$ where t is time, $t \in [0, T] \subset \mathbf{R}$; then we assume that $x(X, t)$ is a homeomorphism of H for all t and that it is continuously differentiable on $H \times [0, T]$; then

$$\frac{\partial}{\partial t} x(X, t) = v(X, t) \tag{1.2}$$

will be called the velocity of point $X \in H$. Since H is identical with its tangent dual space, we assume that $v(X, t) \in H$. Moreover, we assume that the linear operator

$$Dv(X, t) = D\frac{\partial}{\partial t} x(X, t) = \frac{\partial}{\partial t} Dx(X, t) \tag{1.3}$$

is continuous and the mapping $(X, t) \to Dv(X, t)$ is also continuous.

Since $X \to x$ is a homeomorphism, the velocity can be regarded as a function of x, t; then, applying the chain rule, we have

$$Dv = D_x v \circ Dx. \tag{1.4}$$

Let now $Dx^* = Dx^*(X, t)$ be the operator adjoint in the sense of the Hilbert space to Dx, i.e.,

$$\big(Dx(Y)|Z\big) = \big(Y|Dx^*(Z)\big) \tag{1.5}$$

for all $Y, Z \in H$. We recall that $||Dx^*|| = ||Dx||$, $(Dx^*)^* = Dx$, $(Dx^*)^{-1} = (Dx^{-1})^*$.

For arbitrary Dx, i.e., for arbitrary X, t we introduce a linear, continuous, self-adjoint operator $C = C(X, t) = Dx^* \circ Dx$; this operator is positive definite, i.e., for $0 \neq Y \in H$ $(C(Y)|Y) > 0$; furthermore $||C|| = ||Dx||^2$. Then there exists [12] a unique linear continuous operator, called the absolute value of Dx, $\sqrt{C} = |Dx|$, such that $|Dx|^2 = C$; the operator $\sqrt{C}$ is positive and commutes with every operator commuting with Dx. The corresponding notations for Dx^* are the following: $c = Dx \circ Dx^*, \sqrt{c} = |Dx^*|$; we have $||c|| = ||Dx^*||^2 = ||Dx||^2$ and $\sqrt{c}$ commutes with every operator commuting with Dx^*.

We now invoke the polar decomposition theorem [12]: for every Dx there exists a unitary (linear continuous) operator U mapping H onto H such that

$$Dx = U\sqrt{C}. \tag{1.6}$$

For the adjoint operator Dx^*

$$Dx^* = V\sqrt{c}, \tag{1.7}$$

V is also unitary; taking the adjoint relations we obtain

$$Dx^* = \sqrt{C}U^*, \qquad Dx = \sqrt{c}V^*. \tag{1.8}$$

Constructing the operator $Dx \circ Dx^*$, we have

$$Dx \circ Dx^* = c = U \circ \sqrt{C} \circ \sqrt{C} \circ U^* \tag{1.9}$$

i.e.

$$c = U \circ C \circ U^* \tag{1.10}$$

and similarly

$$C = V \circ c \circ V^*. \tag{1.11}$$

Comparing the decompositions of Dx we have

$$\sqrt{c} \circ V^* = U \circ \sqrt{C} \quad \text{i.e.} \quad \sqrt{c} = U \circ \sqrt{C} \circ V, \tag{1.12}$$

whence

$$c = U \circ \sqrt{C} \circ V \circ U \circ \sqrt{C} \circ V, \tag{1.13}$$

Thus, from Eq. (1.10), $V = U^*$ and finally

$$\begin{aligned} Dx &= U \circ \sqrt{C} = \sqrt{c} \circ U, \\ Dx^* &= \sqrt{C} \circ U^* = U^* \circ \sqrt{c} \end{aligned} \tag{1.14}$$

and

$$c = U \circ C \circ U^*, \quad C = U^* \circ c \circ U. \tag{1.15}$$

The polar decomposition of Dx is the counterpart of the decomposition of the deformation gradient in the finite-dimensional Euclidean spaces into the product of the rotation and the strain tensor; we shall call therefore C the right Cauchy–Green strain tensor and c the left Cauchy–Green strain tensor.

1.2. Definition of the divergence of $v(x, t)$ and its properties

Consider the velocity $v(x, t)$. In the case of finite-dimensional space, denoting by $\{\Phi_n\}$, $n = 1, 2, \ldots, N$ the system of base vectors orthogonal, normed and by $(|)$ the scalar product, we have

$$\operatorname{div} v(x) = \sum_{m=1}^{N}\sum_{n=1}^{N}\left(\Phi_n \middle| \frac{\partial v_n}{\partial x^m}\Phi_m\right) = \sum_{n=1}^{N}(\Phi_n|D_x v\Phi_n). \tag{1.16}$$

Thus in the considered Hilbert space we define

$$\operatorname{div} v(x) = \sum_{n=1}^{\infty}(\Phi_n|D_x v\Phi_n) \tag{1.17}$$

where, as before, $\{\Phi_n\}_{n=1}^{\infty}$ is an orthogonal system. We assume that it is complete. We recall that for a linear operator A, $\sum_{n=1}^{\infty}(\Phi_n|A\Phi_n)$ is called the trace of A and denoted by $\operatorname{Tr} A$ or $\operatorname{Sp} A$. In order that this definition be meaningful, we assume that the operator $D_x v$ is nuclear. Then (and only then) [7] the above expression for div $v(x)$ is independent of the choice of $\{\Phi_n\}_{n=1}^{\infty}$ and $\operatorname{div} v(x) < \infty$. Moreover,

$$\operatorname{div} v(x) = \sum_{n=1}^{\infty}\lambda_n, \tag{1.18}$$

where λ_n are the eigenvalues of $D_x v$. Note that since $Dv = D_x v \circ Dx$,

$$\operatorname{div} v(x) = \sum_{n=1}^{\infty}(\Phi_n|Dv \circ Dx^{-1}\Phi_n). \tag{1.19}$$

The expression div $v(x)$ plays an important role in further considerations concerning the Liouville equation.

Introduce now the displacement

$$u = x(X, t) - X = u(X, t) \tag{1.20}$$

which can also be regarded as a function of x and t, and define the linear, continuous, self-adjoint operator

$$E = C - I = Dx^* \circ Dx - I \tag{1.21}$$

or, in terms of the displacement,

$$E = Du + Du^* + Du^* \circ Du. \tag{1.22}$$

We assume now that the operator E is nuclear; then the system of its eigenvectors $\{\Phi_n\}_{n=1}^{\infty}$ is a complete basis in the considered Hilbert space H which we assume to be orthogonal and normalized. The eigenvalues of E

(1.23) $$E\Phi_n = \lambda_n \Phi_n$$

are real and

(1.24) $$\sum_{n=1}^{\infty} \lambda_n < \infty .$$

The operator C has the same system of eigenvectors

(1.25) $$C\Phi_n = (\lambda_n+1)\Phi_n$$

and since C is positive definite,

(1.26) $$\lambda_n+1 > 0.$$

The relation (1.25) can be written in the form

(1.27) $$\psi_n' = \frac{1}{\lambda_n+1}\psi_n,$$

where

(1.28) $$\psi_n = Dx\Phi_n, \quad \psi_n' = (Dx^*)^{-1}\Phi_n.$$

The bases $\{\psi_n\}_{n=1}^{\infty}$, $\{\psi_n'\}_{n=1}^{\infty}$ (in general neither orthogonal nor normalized) will be called biorthogonal, since

(1.29) $$(\psi_m|\psi_n') = (Dx\Phi_m|(Dx^*)^{-1}\Phi_n) = (\Phi_m|\Phi_n) = \delta_{mn}.$$

Let us now differentiate the operator E with respect to time, denoting now the differentiation by a dot; making use of Eqs. (1.4) and (1.21) we have, after transformations,

(1.30) $$\dot{E} = Dx^* \circ 2d \circ Dx,$$

where

(1.31) $$d = \frac{1}{2}(D_x v + D_x v^*)$$

is the rate of the strain operator. We shall later need the "rotation operator"

(1.32) $$\omega = \frac{1}{2}(D_x v - D_x v^*).$$

Furthermore, since $\lambda_n = (\Phi_n|E\Phi_n)$, $(\dot{\Phi}_n|\Phi_n) = 0$ and $E^* = E$

(1.33) $$\dot{\lambda}_n = (\Phi_n|E\Phi_n)^{\boldsymbol{\cdot}} = (\dot{\Phi}_n|E\Phi_n)+(\Phi_n|\dot{E}\Phi_n)+(\Phi_n|E\dot{\Phi}_n)$$
$$= \lambda_n(\dot{\Phi}_n|\Phi_n)+(\Phi_n|\dot{E}\Phi_n)+(E\Phi_n|\dot{\Phi}_n) = (\Phi_n|\dot{E}\Phi_n)$$

and making use of Eq. (1.30),

(1.34) $$\dot{\lambda}_n = (\Phi_n|Dx^* \circ 2d \circ Dx\Phi_n) = 2(Dx\Phi_n|d \circ Dx\Phi_n) = 2\big((\lambda_n+1)\psi_n'|d\psi_n\big)$$

i.e.,

(1.35) $$\frac{1}{2}\frac{\dot{\lambda}_n}{\lambda_n+1} = (\psi_n'|d\psi_n).$$

Since the bases $\{\psi_n\}$, $\{\psi_n'\}$ are biorthogonal, in view of the theorem of invariance of the trace of nuclear operator [7] we obtain

(1.36) $$\operatorname{tr} d = \sum_{n=1}^{\infty} (\psi_n'|d\psi_n) = \sum_{n=1}^{\infty} \ln \sqrt{\dot{\lambda}_n + 1} = \frac{D}{Dt} \ln \prod_{n=1}^{\infty} \sqrt{\lambda_n + 1}.$$

Furthermore, since $\operatorname{tr} D_x v = \operatorname{tr} D_x v^*$, we have, making use of Eq. (1.31),

(1.37) $$\operatorname{div} v = \sum_{n=1}^{\infty} \frac{1}{2} \big((D_x v + D_x v^*)\psi_n|\psi_n'\big) = \operatorname{tr} d,$$

whence

(1.38) $$\operatorname{div} v = \frac{D}{Dt} \ln \prod_{n=1}^{\infty} \sqrt{\lambda_n + 1}.$$

Denoting by

(1.39) $$J = \prod_{n=1}^{\infty} \sqrt{\lambda_n + 1}$$

the counterpart of the Jacobian in the finite-dimensional case, we define the determinant of the operator C as follows:

(1.40) $$\det C = J^2$$

Thus

(1.41) $$\operatorname{div} v = \frac{D}{Dt} \ln J = \frac{D}{Dt} \ln \sqrt{\det C}.$$

Note finally, that the definition (1.28) of the base vector $\{\psi_n\}$ implies the formula

(1.42) $$J = \prod_{n=1}^{\infty} ||\psi_n||.$$

1.3. Hamiltonian velocity

In order to develop the Hamiltonian mechanics and the Liouville theorem, it is important to introduce the Hamiltonian velocity. To this end we first decompose the considered Hilbert phase space into the product of two identical Hilbert spaces

$$H = H' \times H'$$

corresponding in the finite-dimensional case to the decomposition of the $2n$-dimensional phase space into the n-dimensional configuration and momentum spaces. The scalar product, with the obvious notation, is defined as usual in terms of the scalar product in H

$$\big((x_1, y_1)|(x_2, y_2)\big) = (x_1|x_2) + (y_1|y_2),$$

where $(x_1, y_1) \in H' \times H'$, $(x_2, y_2) \in H' \times H'$.

Introduce now the linear operator

(1.43) $$\sigma\colon H' \times H' \to H' \times H'$$

given by

$$\sigma = \begin{bmatrix} 0 & -I \\ I & 0 \end{bmatrix} \tag{1.44}$$

in terms of the unit operator in H; thus, we have

$$\sigma\big((x, y)\big) = (y, -x) \tag{1.45}$$

for $(x, y) \in H' \times H'$. We note that the operator σ is anti-Hermitian, $\sigma^* = -\sigma$ and $\sigma^2 = -I$.

Let now the Hamiltonian $\mathscr{H}$ be a real function of class C^2

$$\mathscr{H}: H' \times H' \times [0, T] \to \mathbf{R}$$

and define the Hamiltonian velocity by the formula

$$v_{\mathscr{H}} = \sigma \circ D_x \mathscr{H}, \tag{1.46}$$

where $D_x\mathscr{H}$ is the Fréchet derivative of $\mathscr{H}$. Thus, if $(q, p) \in H' \times H'$, suppressing the time argument

$$v_{\mathscr{H}}(q, p) = v_{\mathscr{H}} = \big(D_p\mathscr{H}(q, p), -D_q\mathscr{H}(q, p)\big) \tag{1.47}$$

and

$$D_x v_{\mathscr{H}} = \begin{bmatrix} D_{qp}\mathscr{H}(q, p), & D_{pp}\mathscr{H}(q, p) \\ -D_{qq}\mathscr{H}(q, p), & -D_{pq}\mathscr{H}(q, p) \end{bmatrix}, \tag{1.48}$$

The second Fréchet derivatives are linear operators from H' into H'. We now have

THEOREM 1. *If v is a Hamiltonian velocity and $D_x v_{\mathscr{H}}$ is a nuclear operator (from H into H), then* $\operatorname{div} v_{\mathscr{H}} = 0$.

P r o o f. According to the definition

$$\operatorname{div} v = \sum_{n=1}^{\infty} (\Phi_n | D_x v \Phi_n), \tag{1.49}$$

where $\{\Phi_n\}_{n=1}^{\infty}$ is a complete system in H, which can be considered as two systems $\{(e_n, 0)\}_{n=1}^{\infty}$, $\{(0, e_n)\}_{n=1}^{\infty}$ where $\{e_n\}_{n=1}^{\infty}$ is a complete (orthogonal and normalized) system in H'. Thus

$$\operatorname{div} v = \sum_{n=1}^{\infty} \big((e_n, 0) | D_x v(e_n, 0)\big) + \big((0, e_n) | D_x v(0, e_n)\big) \tag{1.50}$$

but

$$D_x v(e_n, 0) = \begin{bmatrix} D_{qp}\mathscr{H}, & D_{pp}\mathscr{H} \\ -D_{qq}\mathscr{H}, & -D_{pq}\mathscr{H} \end{bmatrix} (e_n, 0) = (D_{qp}\mathscr{H} e_n | -D_{qq}\mathscr{H} e_n) \tag{1.51}$$

and

$$D_x v(0, e_n) = \begin{bmatrix} D_{qp}\mathscr{H}, & D_{pp}\mathscr{H} \\ -D_{qq}\mathscr{H}, & -D_{pq}\mathscr{H} \end{bmatrix} (0, e_n) = \big((D_{pp}\mathscr{H} e_n, -D_{pq}\mathscr{H} e_n\big). \tag{1.52}$$

Hence

$$\begin{aligned} \big((e_n, 0) | (D_{qp}\mathscr{H} e_n, -D_{qq}\mathscr{H} e_n)\big) &= (e_n | D_{qp}\mathscr{H} e_n), \\ \big((0, e_n) | (D_{pp}\mathscr{H} e_n, -D_{pq}\mathscr{H} e_n)\big) &= (e_n | -D_{pq}\mathscr{H} e_n) \end{aligned} \tag{1.53}$$

and introducing Eqs. (1.53) into Eq. (1.50), we obtain

$$\text{(1.54)} \qquad \operatorname{div} v = \sum_{n=1}^{\infty} [(e_n | D_{qp}\mathcal{H} e_n) + (e_n| - D_{pq}\mathcal{H} e_n)] = 0$$

since $D_{pq}\mathcal{H} = D_{qp}\mathcal{H}$. Q.E.D.

We now return to kinematic considerations based on the operator σ, which will be used later, in investigating canonical transformations. First, we introduce the anti-Hermitian operators

$$\text{(1.55)} \qquad \begin{aligned} C_\sigma &= Dx^* \circ \sigma \circ Dx, \qquad E_\sigma = C_\sigma - \sigma, \\ c_\sigma &= Dx \circ \sigma \circ Dx^*, \qquad e_\sigma = c_\sigma - \sigma \end{aligned}$$

or, in displacements,

$$\text{(1.56)} \qquad \begin{aligned} E_\sigma &= \sigma \circ Du + Du^* \circ \sigma + Du^* \circ \sigma \circ Du, \\ e_\sigma &= Du \circ \sigma + \sigma \circ Du^* + Du \circ \sigma \circ Du^*. \end{aligned}$$

The time derivatives of the above operators have the form

$$\text{(1.57)} \qquad \dot{C}_\sigma = \dot{E}_\sigma = Dx^* \circ 2\omega_\sigma \circ Dx,$$

where

$$\text{(1.58)} \qquad \begin{aligned} \omega_\sigma &= \frac{1}{2}(\sigma \circ D_x v + D_x v^* \circ \sigma) = \frac{1}{2}\big(\sigma \circ D_x v - (\sigma \circ D_x v)^*\big), \\ \omega_\sigma^* &= -\omega_\sigma. \end{aligned}$$

It is also convenient to use the Hermitian operators

$$\text{(1.59)} \qquad d_\sigma = \frac{1}{2}(\sigma \circ D_x v - D_x v^* \circ \sigma) = \frac{1}{2}\big(\sigma \circ D_x v + (\sigma \circ D_x v)^*\big).$$

Observe that

$$\text{(1.60)} \qquad \omega_\sigma(v) = \omega(\sigma v), \qquad d_\sigma(v) = d(\sigma \circ v).$$

The condition $\omega_\sigma = 0$ is equivalent to the self-adjointness of the operator $\sigma \circ D_x v = D_x(\sigma \circ v)$. Thus, we have the following equivalent statements:

i) v is a Hamiltonian vector field, $v = \sigma \circ D_x\mathcal{H}$,

ii) the operator $D_x(\sigma v)$ is self-adjoint,

iii) $\omega_\sigma = 0$, i.e. $D_x v^* = \sigma \circ D_x v \circ \sigma$,

iv) $\dot{C}_\sigma = 0$.

1.4. Canonical transformations

Define first the Poisson brackets as follows: for the Fréchet differentiable functions $f, g \colon H' \times H' \to R$

$$\text{(1.61)} \qquad \{f, g\} = (D_x f | \delta D_x g)_{H' \times H'},$$

where $x = (q, p)$, $D_x f = (D_q f, D_p f)$, $D_x g = (D_q g, D_p g)$ and by Riesz lemma $D_q f, D_p f, D_q g, D_p g \in H'$. Thus

(1.62) $$(D_x f|\sigma D_x g)_{H'\times H'} = (D_q f, D_p f)|\begin{bmatrix} 0 & -I \\ I & 0 \end{bmatrix}(D_q g, D_p g))_{H'\times H'}$$
$$= ((D_q f, D_p f)|(D_p g, -D_q g))_{H'\times H'} = (D_q f|D_p g)_{H'} - (D_p f|D_q g)_{H'}.$$

The Poisson bracket (1.61) has the same properties as in the finite-dimensional case and reduces to the latter if H is finite-dimensional:

i) it is bilinear,

ii) $\{f, g\} = -\{g, f\}$,

iii) $\{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} = 0$ the Jacobi identity.

We define a canonical transformation $\psi: x \to x$ as follows: for arbitrary f, g

(1.63) $$\{\psi^* \circ f, \psi^* \circ g\} = \{f, g\} \circ \psi^{-1}$$

i.e., omitting the argument ψ^{-1}

(1.64) $$D_x f \circ D\psi^{-1} - \sigma D_x g \circ D\psi^{-1} = D_x f \circ \sigma \circ D_x g$$

or, equivalently,

(1.65) $$\psi^* \circ v_g = v_{\psi^* \circ g}$$

for arbitrary g.

Taking into account that

(1.66) $$D_x g \circ D\psi^{-1} = (D\psi^{-1})^* \circ D_x g,$$

we have our definition in the form

(1.67) $$D\psi \circ \sigma \circ D\psi^* = \sigma$$

i.e.

$$e_\sigma = 0.$$

We note that since $\det \sigma = 1$,

(1.68) $$\det D\psi = \pm 1.$$

In the finite-dimensional case the condition (1.67) has the form

(1.69) $$x^i_{,K} x^j_{,L} \sigma^{KL} = \sigma^{ij}$$

or, decomposing the phase space ($\alpha, \beta, \gamma = 1, \dots, N$),

(1.70) $$\begin{aligned} &\frac{\partial q^\alpha}{\partial Q^\gamma}\frac{\partial q^\beta}{\partial P^\gamma} - \frac{\partial q^\alpha}{\partial P^\gamma}\frac{\partial q^\beta}{\partial Q^\gamma} = 0, &&\frac{\partial q^\gamma}{\partial Q^\alpha}\frac{\partial q^\gamma}{\partial P^\beta} - \frac{\partial q^\gamma}{\partial P^\alpha}\frac{\partial q^\gamma}{\partial Q^\beta} = 0,\\ &\frac{\partial q^\alpha}{\partial Q^\gamma}\frac{\partial p^\beta}{\partial P^\gamma} - \frac{\partial q^\alpha}{\partial P^\gamma}\frac{\partial p^\beta}{\partial P^\gamma} = \delta^{\alpha\beta}, &&\frac{\partial q^\gamma}{\partial Q^\alpha}\frac{\partial p^\gamma}{\partial P^\beta} - \frac{\partial q^\gamma}{\partial P^\beta}\frac{\partial p^\gamma}{\partial Q^\alpha} = \delta_{\alpha\beta},\\ &\frac{\partial p^\alpha}{\partial Q^\gamma}\frac{\partial p^\beta}{\partial P^\gamma} - \frac{\partial p^\alpha}{\partial P^\gamma}\frac{\partial p^\beta}{\partial Q^\gamma} = 0, &&\frac{\partial p^\gamma}{\partial Q^\alpha}\frac{\partial p^\gamma}{\partial P^\beta} - \frac{\partial p^\gamma}{\partial Q^\beta}\frac{\partial p^\gamma}{\partial P^\alpha} = 0 \end{aligned}$$

(summation over γ).

Let us now define the Lie derivative of a smooth scalar function (for an arbitrary velocity v) as follows:

(1.71) $$\mathcal{L}_v f = Dfv.$$

The operator $\mathscr{L}_v \colon F(H) \to F(H)$ is a derivation, i.e., satisfies the following conditions:

i) $\mathscr{L}_v$ is linear

ii) the Leibniz rule holds, i.e.,

$$\mathscr{L}_v(fg) = (\mathscr{L}_v f)g + f(\mathscr{L}_v g). \tag{1.72}$$

Of course, if c is a constant, $\mathscr{L}_v c = 0$. Let us now see how this operator behaves under the diffeomorphism ψ; we have

$$\mathscr{L}_{\psi^* \circ v}(\psi^* \circ f) = \psi^* \circ \mathscr{L}_v f. \tag{1.73}$$

In fact

$$\mathscr{L}_{\psi^* \circ v}(\psi^* \circ f) = D(f \circ \psi^{-1}) \circ D\psi \circ v \circ \psi^{-1} = Df \circ v \circ \psi^{-1} = \psi^* \circ \mathscr{L}_v f. \tag{1.74}$$

We note that for a Hamiltonian velocity v_g, the Poisson bracket (1.61) can be written in the form

$$\{f, g\} = Dfv_g = \frac{dv_g}{dt} f. \tag{1.75}$$

Hence

$$\{f, g\} = \mathscr{L}_{v_g} f. \tag{1.76}$$

Thus the function space $F(H)$ with the composition $\{\ ,\ \}$ is a Lie algebra.

DEFINITION. *The diffeomorphism $\psi \colon H \to H$ is canonical if it preserves the Poisson bracket, i.e,*

$$\{\psi^* \circ f, \psi^* \circ g\} = \psi^* \circ \{f, g\}. \tag{1.77}$$

THEOREM 2. *The diffeomorphism ψ is canonical if and only if for $v_g = \sigma \circ Dg$*

$$\psi^* \circ v_g = v_{\psi^* \circ g}. \tag{1.78}$$

Proof. It follows from the definition (1.77) and from Eqs. (1.73), and (1.76) that

$$\{\psi^* \circ f, \psi^* \circ g\} = \mathscr{L}_{v_{\psi^* \circ g}}(\psi^* \circ f). \tag{1.79}$$

If now $v_{\psi^* \circ g} = \psi^* \circ v_g$,

$$\mathscr{L}_{v_{\psi^* \circ g}}(\psi^* \circ f) = \mathscr{L}_{\psi^* \circ v_g}(\psi^* \circ f) = \psi^* \circ \{f, g\} \tag{1.80}$$

and conversely.

As usual, canonical transformations constitute a group:

THEOREM 3. *The set of canonical transformations with the composition "$\circ$" is a group.*

Proof. The identity is of course canonical. Let now ψ, Φ be canonical; for $\Phi \circ \psi$ we have

$$\{\Phi^* \circ \psi^* \circ f, \Phi^* \circ \psi^* \circ g\} = \Phi^* \circ \{\psi^* \circ f, \psi^* \circ g\} = \Phi^* \circ \psi^* \circ \{f, g\} = (\Phi \circ \psi)^* \circ \{f, g\}. \tag{1.81}$$

It follows also from the above formula that if ψ is canonical, ψ^{-1} is also canonical; it is sufficient to write $\Phi = \psi^{-1}$.

We shall now find the general form of transformations preserving the form of the Hamilton equations. Let $x \to y$ be a diffeomorphism of H. We have the Hamilton equations

$$\dot{x} = \sigma D_x \mathscr{H},$$

(1.82)
$$\dot{y} = D_x y \dot{x} + \frac{\partial y}{\partial t}.$$

We require that

(1.83)
$$\dot{y} = \sigma D_y \mathscr{H}',$$

where $\mathscr{H}'$ is a Hamiltonian; thus we must have

(1.84)
$$\sigma \circ \left(D_x y \dot{x} + \frac{\partial y}{\partial t} \right) = -D_y \mathscr{H}' \quad \text{or} \quad \sigma \left(D_x y \circ \sigma \circ D_x \mathscr{H} + \frac{\partial y}{\partial t} \right) = -D_y \mathscr{H}'$$

and hence it is necessary and sufficient that the linear operator [2]

(1.85)
$$D_y \left[\sigma \circ \left(D_x y \circ \sigma \circ D_x \mathscr{H} + \frac{\partial y}{\partial t} \right) \right]$$

be self-adjoint for arbitrary $\mathscr{H}$. It follows that the operators in (1.85) containing different derivatives of $\mathscr{H}$ must also be self-adjoint.

(1.86)
$$D_y \left(\sigma \circ \frac{\partial y}{\partial t} \right) = D_y \left(\sigma \circ \frac{\partial y}{\partial t} \right)^*$$

i.e.

(1.87)
$$D_x \left(\sigma \circ \frac{\partial y}{\partial t} \right) D_y x = \left[D_x \left(\sigma \circ \frac{\partial y}{\partial t} \right) D_y x \right]^*$$

or

(1.88)
$$\sigma \circ \frac{\partial}{\partial t} D_x y \circ D_y x = -D_y x \circ \frac{\partial}{\partial t} D_x y \circ \sigma.$$

Multiplying on the left by $D_x y^*$ and on the right by $D_x y$, we obtain

(1.89)
$$\frac{\partial}{\partial t} C_\sigma = 0,$$

where $C_\sigma = Dx^* \circ \sigma \circ Dx$(1) is the anti-Hermitian operator introduced in Eqs. (1.55).

Since $D_x \mathscr{H}$ or $\sigma \circ D_x \mathscr{H}$ is arbitrary

(1.90)
$$\sigma \circ D_x D_x y \circ D_y x = D_y x^* \circ D_x (D_x y)^* \circ \sigma^*.$$

and multiplying as in Eq. (1.88), we have

(1.91)
$$D_x C_\sigma = 0.$$

The condition for the second derivatives is

(1.92)
$$\sigma \circ D_x y \circ \sigma \circ D_x D_x \mathscr{H} \circ D_y x = (\sigma \circ D_x y \circ \sigma \circ D_x D_x \mathscr{H} \circ D_y x)^*$$

or, after simple transformations,

(1.93)
$$C_\sigma \circ \sigma \circ D_x D_x \mathscr{H} = D_x D_x \mathscr{H} \circ \sigma \circ C_\sigma$$

and $D_x D_x \mathscr{H}$ being arbitrary

(1.94)
$$C_\sigma = \mu \sigma,$$

(1) More precise notation is $C_{\sigma, x \to y}$

where $\mu \in R$. In view of Eqs. (1.89) and (1.91) μ is a constant real number. Finally, taking into account the fact that the identity is a canonical transformation, we obtain $\mu = 1$. Thus the required condition is

$$C_\sigma = \sigma. \tag{1.95}$$

2. The variational principle and the equations of motion

2.1. The du Bois-Raymond lemma in Hilbert space

Let $f(\cdot, t)$ be a linear continuous functional on Hilbert space H depending on the real parameter t, and let $h(t) \in H$; then $f(h(t), t) \in R$. We assume that both $h(t)$ and $f(\cdot, t)$ are continuous in t. By this assumptions we have the following

LEMMA. If

$$\int_{t_1}^{t_2} dt f\big(h(t), t\big) = 0 \tag{2.1}$$

for an arbitrary $h(t) \in H$ satisfying the boundary conditions $h(t_1) = h(t_2) = 0$, then

$$f\big(h(t), t\big) = 0 \quad \text{for} \quad t \in [t_1, t_2]. \tag{2.2}$$

Proof. According to the Riesz lemma, the considered functional has the form of a scalar product

$$f\big(h(t), t\big) = \big(a(t)|h(t)\big), \tag{2.3}$$

where $a(t) \in H$ is uniquely determined by f, and $||f|| = ||a||$. Furthermore, $a(t)$ is continuous in t. Let for a $\tau \in [t_1, t_2]$ $a(\tau) \neq 0$, then $a(t) \neq 0$ in a certain neighbourhood of τ i.e., in $[\tau-\varepsilon, \tau+\varepsilon]$. Additionally we assume that for $s \in [\tau-\varepsilon, \tau+\varepsilon]$,

$$\big(a(s)|a(\tau)\big) > \beta > 0. \tag{2.4}$$

Now we choose in this region

$$h(t) = a(\tau)\varphi(t) \tag{2.5}$$

where $\varphi(t_1) = \varphi(t_2) = 0$, $\varphi(t)$ is continuous, $\operatorname{supp}\varphi \subset [\tau-\varepsilon, \tau+\varepsilon]$ and $\varphi(\tau) > 0$. Then

$$\int_{t_2}^{t_1} dt f\big(h(t), t\big) = \int_{t_1}^{t_2} dt \big(a(t)|h(t)\big) \geqslant \int_{\tau-\varepsilon}^{\tau+\varepsilon} dt \beta\varphi(t) > 0 \tag{2.6}$$

which contradicts the assumption. Hence $a(t) = 0$ and therefore $f(h(t), t) = 0$ for $t \in [t_1, t_2]$.

REMARK. It is easy to see that the above lemma holds even in the case when the functions $h(t)$ are of class C^∞ with compact support and $h(t_1) = h(t_2) = 0$. Observe that in the finite-dimensional case it is sufficient to assume that only the functions $h(t)$ and $f(h(t), t)$ are continuous in t.

2.2. The equations of motion. Passing from Lagrangian to Hamiltonian mechanics

Now we are in a position to proceed to the Hamilton principle. Consider the Lagrangian functional $L: H \times H \times [t_1, t_2] \to R$ or $L(q(t), \dot{q}(t), t) \in R$ and introduce new vectors $(\delta q(t), \delta\dot{q}(t)) \in H \times H$, where

$$\delta\dot{q}(t) = \delta\frac{dq(t)}{dt} = \frac{d}{dt}\delta q(t). \tag{2.7}$$

Assuming that the Fréchet derivative of L exists and is continuous ([2]) on $H\times H$, we have

$$L(q+\delta q, q+\delta\dot{q}, t) - L(q, \dot{q}, t) = DL\circ(\delta q, \delta\dot{q}) + r, \tag{2.8}$$

where

$$\frac{||r||}{||\delta q||+||\delta\dot{q}||} \to 0 \quad \text{as} \quad ||\delta q||+||\delta\dot{q}|| \to 0.$$

The action of the linear continuous functional DL in $H\times H$ can be written in the form

$$DL\circ(\delta q, \delta\dot{q}) = D_q L\circ\delta q + D_{\dot{q}} L\circ\delta\dot{q}, \tag{2.9}$$

where $D_q L$ and $D_{\dot{q}} L$ are partial Fréchet derivatives. The quantity in the left-hand side of the above equation will be called the variation of L, i.e., $\delta L = DL\circ(\delta q, \delta\dot{q})$. We have

$$D_{\dot{q}} L\circ\delta\dot{q} = D_{\dot{q}} L\frac{d}{dt}\delta q = \frac{d}{dt}(D_{\dot{q}} L\circ\delta q) - \frac{d}{dt}D_{\dot{q}} L\circ\delta q. \tag{2.10}$$

Consider now a smooth trajectory C and the action functional

$$A[C] = \int_{t_1}^{t_2} dt L(q(t), \dot{q}(t), t). \tag{2.11}$$

Let C' be another trajectory with different, in general, end points and denote the variations

$$\begin{gathered} t_1' - t_1 = \delta t_1, \quad t_2' - t_2 = \delta t_2, \\ q'(t) = q(t) + \delta q. \end{gathered} \tag{2.12}$$

Observe that

$$\dot{q}'(t) = \dot{q}(t) + \frac{d}{dt}\delta q(t). \tag{2.13}$$

We are interested in the variation of the action functional

$$\delta A = A[C'] - A[C] = \int_{t_1}^{t_2} dt L(q'(t), \dot{q}'(t), t) - \int_{t_1}^{t_2} dt L(q(t), \dot{q}(t), t), \tag{2.14}$$

Making use of Eqs. (2.8), (2.9) and (2.10), we obtain

$$\begin{aligned} \delta A &= \int_{t_1}^{t_2} dt \left[\left(D_q L - \frac{d}{dt}D_{\dot{q}} L\right)\circ\delta q + \frac{d}{dt}(D_{\dot{q}} L\circ\delta q)\right] + L\delta t\Big|_{t_1}^{t_2} \\ &= \int_{t_1}^{t_2} dt \left(D_q L - \frac{d}{dt}D_{\dot{q}} L\right)\circ\delta q + (L\delta t + D_q L\circ\delta q)\Big|_{t_1}^{t_2}. \end{aligned} \tag{2.15}$$

We shall state the Hamilton principle as follows: for variations of trajectories with fixed end points, i.e., $\delta t = 0$, and $\delta q = 0$ at the end points,

$$\delta A = \int_{t_1}^{t_2} dt \left(D_q L - \frac{d}{dt}D_{\dot{q}} L\right)\circ\delta q = 0 \tag{2.16}$$

([2]) This assumption is needed only later.

for arbitrary variations δq, continuous in t and vanishing at t_1 and t_2.

The du Bois–Raymond lemma implies for $t \in [t_1, t_2]$ the Lagrange equations of motion

$$D_q L - \frac{d}{dt} D_{\dot{q}} L = 0 \tag{2.17}$$

for the considered system described by the trajectory $q(t)$ in the Hilbert space H. These equations state that for the real trajectory the element of H^* given by the left-hand side of Eq. (2.17) vanishes.

Performing the differentiation we have the equation

$$D_{\dot{q}} D_{\dot{q}} L \circ \ddot{q} + D_q D_{\dot{q}} L \circ \dot{q} - D_q L + \frac{\partial}{\partial t} D_{\dot{q}} L = 0 \tag{2.18}$$

containing explicitly the acceleration $\ddot{q}(t)$.

In passing from Lagrangian to Hamiltonian mechanics, the basis is the invertibility of the relation $\dot{q} \to D_{\dot{q}} L = p$ between the linear momentum p and the velocity $\dot{q}$. The definition $p = D_{\dot{q}} L$ is in general a nonlinear map of H into H, for a fixed q. In accordance with the inverse function theorem we have the following result: if for a certain $\dot{q}_0 \in H$ the map $D_{\dot{q}}(D_{\dot{q}} L(q, \dot{q}_0))$ is a linear homeomorphism of H into H^*, then there exists an open neighbourhood $\mathcal{U}(\dot{q}_0) \subset H$ in which the map $\dot{q} \to D_{\dot{q}} L(q, \dot{q})$ is a homeomorphism onto a neighbourhood $\mathcal{V}(p_0)$ of $p_0 = D_{\dot{q}} L(q, \dot{q}_0)$ in H. Moreover, if the map $\dot{q} \to D_{\dot{q}} L(q, \dot{q})$ is continuously Fréchet differentiable m times in $\mathcal{U}(q_0)$, then the inverse map has the same property in $\mathcal{V}(p_0)$.

Observe that the condition that $D_{\dot{q}}(D_{\dot{q}} L(q, \dot{q}))$ is a linear isomorphism ensures that the acceleration $\ddot{q}$ is uniquely determined in terms of q and $\dot{q}$ from the Lagrange equations of motion (2.17).

We are now in a position to perform the transition from Lagrange mechanics to Hamilton mechanics. We can write the Lagrange equations of motion in the form

$$p = D_{\dot{q}} L, \quad \dot{p} = D_q L \tag{2.19}$$

the first equation being the definition of the linear momentum and the second the equation of motion. We assume that there exists a function $\tilde{\mathcal{H}}(q, p, t)$ such that

$$D_q L = -D_q \tilde{\mathcal{H}} \tag{2.20}$$

so that

$$\dot{p} = -D_q \tilde{\mathcal{H}}. \tag{2.21}$$

Thus, for $(a, b, \tau) \in H \times H \times R$,

$$\begin{aligned} D\tilde{\mathcal{H}}(a, b) &= D_q \tilde{\mathcal{H}}(a) + D_p \tilde{\mathcal{H}}(b) + \frac{\partial}{\partial t} \tilde{\mathcal{H}}(\tau), \\ DL(a, a') &= D_q L(a) + D_{\dot{q}} L(a') + \frac{\partial}{\partial t} L(\tau). \end{aligned} \tag{2.22}$$

In view of Eqs. (2.20), (2.21) and (2.22), we have

$$D\tilde{\mathcal{H}}(a, b) + DL(a, a') = D_p \tilde{\mathcal{H}}(b) + p(a') + \frac{\partial}{\partial t} (\tilde{\mathcal{H}} + L)(\tau). \tag{2.23}$$

Since $D(p(\dot{q}))(b, a') = p(a') + \dot{q}b$, we determine from this relation the quantity $p(a')$; introducing the total derivative D^T on the space $H \times H \times H \times R$, we obtain

$$D^T(\tilde{\mathscr{H}} + L - p\dot{q})(a, a', b, \tau) = (D_p\tilde{\mathscr{H}} - \dot{q})(b) + \frac{\partial}{\partial t}(\tilde{\mathscr{H}} + L)(\tau). \tag{2.24}$$

Since the elements a, a' and b are arbitrary, it follows that there exists a function $f: H^* \times [t_1, t_2] \to R$ such that

$$\tilde{\mathscr{H}} + L - p(\dot{q}) = f, \quad D_p\tilde{\mathscr{H}} - \dot{q} = D_p f, \quad \frac{\partial}{\partial t}(\tilde{\mathscr{H}} + L) = \frac{\partial}{\partial t} f \tag{2.25}$$

or, introducing the Hamiltonian

$$\mathscr{H}(q, p, t) = \tilde{\mathscr{H}} - f. \tag{2.26}$$

We have

$$\begin{gathered} \mathscr{H}(q, p, t) = p\dot{q} - L(q, \dot{q}, t), \\ D_p\mathscr{H} = \dot{q}, \quad \frac{\partial \mathscr{H}}{\partial t} = -\frac{\partial L}{\partial t}, \end{gathered} \tag{2.27}$$

where $p\dot{q} = p(\dot{q}) = (p|\dot{q})_H$ by the identification of H and H^*. Thus, finally we have the definition of the Hamiltonian

$$\mathscr{H}(q, p, t) = p\dot{q} - L(q, \dot{q}, t) \tag{2.28}$$

and the Hamiltonian equation of motion

$$\dot{q} = D_p\mathscr{H}, \quad \dot{p} = -D_q\mathscr{H}. \tag{2.29}$$

2.3. Examples of the invertibility of the dependence $p(\dot{q})$

Let us assume that

$$L(q, \dot{q}) = K(\dot{q}) - W(q) \quad \text{and} \quad W(q) = 0, \tag{2.30}$$

EXAMPLE 1

$$K(\dot{q}) = \frac{m}{2}(\dot{q}|\dot{q}) = \frac{m}{2}||\dot{q}||^2, \tag{2.31}$$

$$D_{\dot{q}}L(h) = m(\dot{q}|h), \quad h \in H, \tag{2.32}$$

$$p = D_{\dot{q}}L(q, \dot{q}) = m\dot{q}. \tag{2.33}$$

EXAMPLE 2

$$K(\dot{q}) = \frac{m}{4}(\dot{q}|\dot{q})^2, \tag{2.34}$$

$$D_{\dot{q}}L(q, \dot{q}) = m||\dot{q}||^2(\dot{q}|\cdot), \tag{2.35}$$

$$p = m||\dot{q}||^2\dot{q}. \tag{2.36}$$

EXAMPLE 3

(2.37) $$K(\dot{q}) = mc^2\left(1-\sqrt{1-c^{-2}(\dot{q}|\dot{q})}\right),$$

(2.38) $$D_{\dot{q}}L(q,\dot{q})(h) = \frac{(m\dot{q}|h)}{\sqrt{1-c^{-2}(\dot{q}|\dot{q})}},$$

(2.40) $$p = \frac{m\dot{q}}{\sqrt{1-c^{-2}(\dot{q}|\dot{q})}}.$$

EXAMPLE 4

(2.41) $$K(\dot{q}) = (\dot{q}|A\dot{q}),$$

where A is a linear self-adjoint continuous operator $A:H \to H$,

(2.42) $$D_{\dot{q}}L(q,\dot{q})(h) = \frac{m}{2}(\dot{q}|Ah)+(h|A\dot{q}) = \frac{m}{2}\left((A+A^*)\dot{q}|h\right),$$

(2.43) $$p = mA^+\dot{q},$$

where

(2.44) $$A^+ = \frac{1}{2}(A+A^*).$$

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