

## CHAPTER 1

### THE LIOUVILLE EQUATION IN CLASSICAL MECHANICS

#### 1. INTRODUCTION: STATISTICAL APPROACH IN CLASSICAL AND QUANTUM MECHANICS

In both quantum and classical mechanics, evaluation of the states of a dynamical system is deterministic. The states of the system at all times  $t$  are completely determined by the dynamical state at an initial time  $t_0$ .

The fundamental difference between classical and quantum mechanics is in principally different formulations of such basic concepts as the state of a dynamical system and its dynamical variables.

In classical mechanics, a state  $\Omega$  of a dynamical system with  $n$  degrees of freedom is specified by its  $n$  coordinates and  $n$  momenta.

Possible states  $\Omega = (q_1, \dots, q_n; p_1, \dots, p_n)$  are usually considered in a  $2n$ -dimensional phase space.

Evolution of  $\Omega$  in time is specified by the Hamilton canonical equations

$$\frac{\partial q_k}{\partial t} = \frac{\partial p_k}{\partial t}, \quad \frac{\partial p_k}{\partial t} = \frac{\partial q_k}{\partial t}, \quad k = 1, 2, \dots, n, \quad (1.1)$$

where  $H$  is a Hamiltonian of the system. The Hamiltonian is a real function of  $\Omega$

$$H = H(t; q_1, \dots, q_n; p_1, \dots, p_n). \quad (1.2)$$

For a dynamical system which is isolated from external influence, the Hamiltonian does not explicitly depend on  $t$

$$H = H(q_1, \dots, q_n; p_1, \dots, p_n). \quad (1.3)$$

In the framework of classical mechanics, a dynamical variable  $A$  is a function of the dynamical state

$$A = A(\Omega) = A(q_1, \dots, q_n; p_1, \dots, p_n) \quad (1.4)$$

Dynamical variable  $A$  is completely determined by state  $\Omega$ . For simplicity, we restrict the consideration to the dynamical quantities which do not explicitly depend on time.

However in quantum mechanics, the concepts of dynamical state and dynamical variable are introduced in an entirely different way. The state of a dynamical system is specified by a wave function  $\varphi$ , which can be considered as a vector in some Hilbert space. We shall as usual denote the scalar products of two such vectors as

$$(\varphi_1, \varphi_2). \quad (1.5)$$

The evolution of a dynamical state is specified by the Schroedinger wave equation

$$i\hbar \frac{\partial \varphi}{\partial t} = H_t \varphi \quad (1.6)$$

where  $H_t$  is the Hamiltonian of the system under consideration. The Hamiltonian is a linear self-conjugated operator which acts on wave functions  $\varphi$ .

In quantum mechanics, dynamical variables are not functions of the dynamical state. They are linear operators which act on wave functions  $\varphi$ .

Thus, the dynamical state of a system under consideration does not generally speaking specify values of a given dynamical variable which can be experimentally measured.

Only if  $\varphi$  is an eigenfunction of operator  $A$ , i.e., if

$$A\varphi = a\varphi \quad (1.7)$$

where  $a$  is a complex number, can we say that by measuring quantity  $A$  in the state  $\varphi$  we get a definite value  $a$  [3].

In the general case, the dynamical state only determines the expectation value  $\langle A \rangle$  of a dynamical variable  $A$ . So, if we normalize  $(\varphi, \varphi) = 1$  the wave function  $\varphi$  which represents a given dynamical state, the expectation value is given by the known formula

$$\langle A \rangle = (\varphi, A\varphi). \quad (1.8)$$

It should be noted that, in problems of statistical mechanics we deal with dynamical systems consisting of a large or, as the say, macroscopic number  $N$  of interacting particles. For this reason, neither in the framework classical

mechanics nor in the framework of quantum mechanics, is the study of the evolution of each individual dynamical state possible in practice.

In fact, in classical mechanics, for a dynamical system consisting of  $N$  particle, we have

$$\Omega = (\mathbf{q}_1, \dots, \mathbf{q}_n; \mathbf{p}_1, \dots, \mathbf{p}_n) \quad (1.9)$$

where  $\mathbf{q}_j$  and  $\mathbf{p}_j$  are three-dimensional vectors specifying the position and momentum of the  $j$ -th particle. The total number of degrees of freedom is  $n = 3N$ .

In quantum mechanics, a state of system is specified by a wave function

$$\varphi = \varphi(\mathbf{X}) \quad (1.10)$$

where  $\mathbf{X}$  is, for example, a set  $\mathbf{q}_1, \dots, \mathbf{q}_n$ . The set can also contain discrete spin variables. It is clear that the actual construction of both the phase trajectory  $\Omega(t)$  in  $6N$ -dimensional phase space and the wave function  $\varphi(t, \mathbf{X})$ , which depend on time and nor fewer than  $3N$  arguments, is so unrealistic at macroscopic values of  $N$  that it is essential to use a statistical approach [1]. Below we shall successively introduce the basic concepts of such an approach both in classical and quantum mechanics.

## 2. THE CLASSICAL STATISTICAL APPROACH

### a) A Transformation Operator $G$

We shall first consider the case of dynamical systems of classical mechanics and turn to basic equations of motion (1.1). These equations determine a point  $\Omega(t)$  in the phase space as a function of its initial state  $\Omega_0$  at a certain time  $t = t_0$

$$\Omega(t) = G_{t, t_0}(\Omega_0), \quad \Omega_0 = G_{t_0, t_0}(\Omega_0). \quad (1.11)$$

It is clear that we can consider  $G_{t, t_0}$  as a transformation in phase space, mapping a point  $\Omega_0$  to  $\Omega(t)$  in the same space.

Let us make some remarks concerning transformation  $G$ . Since any time can be considered as initial, Equation (1.11) yields

$$\Omega(t_2) = G_{t_2, t_1}(\Omega(t_1)) = G_{t_2, t_1}(G_{t_1, t_0}(\Omega_0))$$

and  $\Omega(t_2) = G_{t_2, t_0}(\Omega_0)$ . We see that right-hand sides of these equations coincide for any positions  $\Omega_0$  in the phase space. We may then omit index 0

and write

$$G_{t_2, t_0}(\Omega) = G_{t_2, t_1}(G_{t_1, t_0}(\Omega)). \quad (1.12)$$

This identity is valid in the whole phase space and also for any of  $t_0$ ,  $t_1$  and  $t_2$ .

Let us make, in particular,  $t_2 = t_0$ ,  $t_1 = t$ . Since  $G_{t_0, t_0}(\Omega) = \Omega$ , Equation (1.12) becomes

$$\Omega = G_{t_0, t}(G_{t, t_0}(\Omega)). \quad (1.13)$$

Since  $t_0$  and  $t$  are completely arbitrary, in Equation (1.13) we can redenote  $t_0$  and  $t$  as  $t$  and  $t_0$ , respectively. Hence, we can also write

$$\Omega = G_{t, t_0}(G_{t_0, t}(\Omega)). \quad (1.14)$$

From Equations (1.13) and (1.14) we conclude that transformations  $G_{t, t_0}$  and  $G_{t_0, t}$  are mutually inverse

$$G_{t, t_0} = G_{t_0, t}^{-1}, \quad G_{t_0, t} = G_{t, t_0}^{-1}. \quad (1.15)$$

## b) Probability Density $\mathcal{D}$

With this in mind, let us introduce some distribution in the phase space at an initial time  $t_0$ . Let  $\mathcal{D}_0(\Omega)$  be the probability density of this distribution, so that the product

$$\mathcal{D}_0 d\Omega = \mathcal{D}_0(q_1, \dots, q_n; p_1, \dots, p_n) dq_1 \dots dq_n dp_1 \dots dp_n$$

gives the probability of finding the initial state  $\Omega = \Omega_0$  in infinitesimal  $6N$ -dimensional volume element  $d\Omega$ . By definition

$$\mathcal{D}_0(\Omega) \geq 0, \quad \int \mathcal{D}_0(\Omega) d\Omega = 1. \quad (1.16)$$

Let us consider a dynamical variable  $A = A(\Omega)$ . In view of Equation (1.11), its value at time  $t$  is

$$A_t = A(G_{t, t_0}(\Omega_0)), \quad (1.17)$$

and therefore its expectation value is given by the integral

$$\langle A_t \rangle = \int A(G_{t, t_0}(\Omega_0)) \mathcal{D}_0(\Omega_0) d\Omega_0. \quad (1.18)$$

In this context, we proceed to study of integral of the form

$$\int F(G_{t,t_0}(\Omega_0))\mathcal{D}_0(\Omega_0)d\Omega_0. \tag{1.19}$$

In this treatment we shall not take into account the normalization condition (1.16). Due to the identity

$$F(G_{t,t_0}(\Omega_0)) = \int \delta(G_{t,t_0}(\Omega_0) - \Omega)F(\Omega)d\Omega$$

where

$$\delta(\bar{\Omega} - \Omega) = \prod_{1 \leq j \leq n} \delta(\bar{q}_j - q_j)\delta(\bar{p}_j - p_j),$$

we can represent the integral in the Equation (1-1.19) in the form

$$\int F(\Omega)\mathcal{D}_{t,t_0}(\Omega)d\Omega$$

where

$$\mathcal{D}_{t,t_0}(\Omega) = \int \delta(G_{t,t_0}(\Omega_0) - \Omega)\mathcal{D}_0(\Omega_0)d\Omega_0. \tag{1.20}$$

In particular, we have

$$\mathcal{D}_{t_0,t_0}(\Omega) = \int \delta(\Omega_0 - \Omega)\mathcal{D}_0(\Omega_0)d\Omega_0 = \mathcal{D}_0(\Omega). \tag{1.21}$$

Thus, on remaining the integration variable  $\Omega_0 \rightarrow \Omega$  in Equation (1.19), we obtain

$$\int F(G_{t,t_0}(\Omega))\mathcal{D}_0(\Omega)d\Omega = \int F(\Omega)\mathcal{D}_{t,t_0}(\Omega)d\Omega. \tag{1.22}$$

### c) The Liouville Theorem

Let us now find a convenient expression for  $\partial/\partial t \mathcal{D}_{t,t_0}(\Omega)$ . We represent the basis equations of motion in a condensed form

$$\frac{\partial \Omega}{\partial t} = \Phi(t, \Omega) \tag{1.23}$$

where

$$\Phi(t, \Omega) = \left\{ \frac{\partial H}{\partial p_1}, \dots, \frac{\partial H}{\partial p_n}; -\frac{\partial H}{\partial q_1}, \dots, -\frac{\partial H}{\partial q_n} \right\}. \tag{1.24}$$

Thus, Equation (1.11) gives

$$\frac{\partial G_{t,t_0}(\Omega_0)}{\partial t} = \Phi(t, G_{t,t_0}(\Omega)). \quad (1.25)$$

Differentiating Equation (1.20) with respect to  $t$ , we find

$$\frac{\partial}{\partial t} \mathcal{D}_{t,t_0}(\Omega_0) = \int \Phi(t, \Omega_1) \frac{\partial}{\partial \Omega_1} \delta(\Omega_1 - \Omega) \mathcal{D}_0(\Omega_0) d\Omega_0$$

where, for brevity, we have put  $\Omega_1 = G_{t,t_0}(\Omega_0)$ . On the other hand, we have

$$\begin{aligned} \Phi(t, \Omega_1) \frac{\partial}{\partial \Omega_1} \delta(\Omega_1 - \Omega) \\ = -\frac{\partial}{\partial \Omega} \Phi(t, \Omega_1) \delta(\Omega_1 - \Omega) = -\frac{\partial}{\partial \Omega} \Phi(t, \Omega) \delta(\Omega_1 - \Omega), \end{aligned}$$

and therefore,

$$\frac{\partial}{\partial t} \mathcal{D}_{t,t_0}(\Omega) = -\frac{\partial}{\partial \Omega} \Phi(t, \Omega) \int \delta(G_{t,t_0}(\Omega_0) - \Omega) \mathcal{D}_0(\Omega_0) d\Omega_0,$$

i.e.,

$$\frac{\partial \mathcal{D}_{t,t_0}(\Omega)}{\partial t} = -\frac{\partial}{\partial \Omega} \Phi(t, \Omega) \mathcal{D}_{t,t_0}(\Omega). \quad (1.26)$$

Taking into account Equation (1.24), we can write this equation in a more detailed form

$$\frac{\partial \mathcal{D}_{t,t_0}}{\partial t} = - \sum_{1 \leq j \leq n} \left\{ \frac{\partial}{\partial q_j} \left( \frac{\partial H}{\partial p_j} \mathcal{D}_{t,t_0} \right) - \frac{\partial}{\partial p_j} \left( \frac{\partial H}{\partial q_j} \mathcal{D}_{t,t_0} \right) \right\}.$$

Upon simplification, we obtain the Liouville equation [1]

$$\frac{\partial \mathcal{D}_{t,t_0}}{\partial t} = - \sum_{1 \leq j \leq n} \left( \frac{\partial H}{\partial p_j} \frac{\partial \mathcal{D}_{t,t_0}}{\partial q_j} - \frac{\partial H}{\partial q_j} \frac{\partial \mathcal{D}_{t,t_0}}{\partial p_j} \right) \quad (1.27)$$

where

$$H = H(t; q_1, \dots, q_n; p_1, \dots, p_n) \quad (1.28)$$

and

$$\mathcal{D}_{t,t_0} = \mathcal{D}_0(q_1, \dots, q_n; p_1, \dots, p_n) = \mathcal{D}_0(\Omega) \quad \text{for } t = t_0. \quad (1.29)$$

Equation (1.29) shows, if we take  $\mathcal{D}_0(\Omega) = 1$  as the initial function, then  $\mathcal{D}_{t,t_0}(\Omega) = 1$ . Substituting this expression into Equation (1.22), we get the identity

$$\int F(G_{t,t_0}(\Omega))d\Omega = \int F(\Omega)d\Omega. \tag{1.30}$$

Let  $\mathcal{G}$  be a finite region in phase space. In the Equation (1.30), we take the characteristic function of this region as  $F$ , i.e., we put

$$F(\Omega) = 1, \quad \Omega \in \mathcal{G}; \quad F(\Omega) = 0, \quad \Omega \notin \mathcal{G}.$$

Then, since  $G_{t_0,t}$  is the inverse transformation to  $G_{t,t_0}$ , we get

$$F(G_{t,t_0}(\Omega)) = 1, \quad \Omega \in G_{t,t_0}\mathcal{G}; \quad F(G_{t,t_0}(\Omega)) = 0, \quad \Omega \notin G_{t,t_0}\mathcal{G}.$$

Here,  $G_{t,t_0}\mathcal{G}$  denotes a region in the phase space which is the image of element  $\mathcal{G}$  under the transformation  $G_{t,t_0}$ . It is now clear that the Liouville volumes of regions  $\mathcal{G}$  and  $G_{t,t_0}\mathcal{G}$  are equal

$$\int_{G_{t_0,t}\mathcal{G}} d\Omega = \int_{\mathcal{G}} d\Omega, \quad d\Omega = dq_1 \dots dq_n dp_1 \dots dp_n.$$

Since  $t$  and  $t_0$  are arbitrary, we can redenote  $t \rightarrow t_0, \quad t_0 \rightarrow t$  and write

$$\int_{G_{t,t_0}\mathcal{G}} d\Omega = \int_{\mathcal{G}} d\Omega. \tag{1.31}$$

We see that  $G_{t,t_0}\mathcal{G}$  is the region occupied at time  $t$  by those and only those points of the phase space which at time  $t_0$  occupied region  $\mathcal{G}$ .

Thus, Equation (1.31) is the well known theorem on conservation of the Liouville phase volume under the motion specified by Equation (??).

#### d) Time Dependent Probability Density $\mathcal{D}_{t,t_0}$

Let us now put in Equation (1.22)  $F(\Omega) = 1$ . We then obtain

$$\int \mathcal{D}_{t,t_0}(\Omega)d\Omega = \int \mathcal{D}_0(\Omega)d\Omega.$$

Then taking into account definition (1.20) and condition (1.16) we find

$$\mathcal{D}_{t,t_0}(\Omega) \geq 0, \quad \int \mathcal{D}_{t,t_0}(\Omega) d\Omega = 1. \quad (1.32)$$

In view of Equations (1.18) and (1.22), we can write

$$\langle A_t \rangle = \int A(G_{t,t_0}(\Omega)) \mathcal{D}_0(\Omega) d\Omega = \int A(\Omega) \mathcal{D}_{t,t_0}(\Omega) d\Omega. \quad (1.33)$$

We thus see that function  $\mathcal{D}_{t,t_0}(\Omega) d\Omega$  represent the probability density at time  $t$ . It has already been mentioned that this function satisfies the Liouville equation (1.27) and the initial condition (1.29).

Introducing the classical Poisson brackets

$$[A, B] = \sum_{1 \leq j \leq n} \left\{ \frac{\partial A}{\partial q_j} \frac{\partial B}{\partial p_j} - \frac{\partial A}{\partial p_j} \frac{\partial B}{\partial q_j} \right\} \quad (1.34)$$

for two arbitrary functions  $A = A(\Omega)$  and  $B = B(\Omega)$  of points  $\Omega$  in the phase space, we can represent the Liouville equation in the form

$$\frac{\partial \mathcal{D}_{t,t_0}}{\partial t} = [H, \mathcal{D}_{t,t_0}]. \quad (1.35)$$

Let us now consider Equation (1.30) and put  $F(\Omega) = A(\Omega) \mathcal{D}_0(G_{t_0,t}(\Omega))$ . Then we have  $F(G_{t,t_0}(\Omega)) = A(G_{t,t_0}(\Omega)) \mathcal{D}_0(\Omega)$ , and therefore,

$$\int A(G_{t,t_0}(\Omega)) \mathcal{D}_0(\Omega) d\Omega = \int A(\Omega) \mathcal{D}_0(G_{t_0,t}(\Omega)) d\Omega. \quad (1.36)$$

Taking into account Equation (1.33), we get

$$\int A(\Omega) \mathcal{D}_{t,t_0}(\Omega) d\Omega = \int A(\Omega) \mathcal{D}_0(G_{t_0,t}(\Omega)) d\Omega.$$

Since function  $A(\Omega)$  is arbitrary, we finally obtain

$$\mathcal{D}_{t,t_0}(\Omega) = \mathcal{D}_0(G_{t_0,t}(\Omega)). \quad (1.37)$$

### 3. QUANTUM ANALOGY

We now consider a linear operator  $S_{t,t_0}$  which transforms an arbitrary function  $f(\Omega)$  of a dynamical state into the function

$$S_{t,t_0}f(\Omega) = f(G_{t,t_0}(\Omega)).$$

We see that

$$\mathcal{D}_{t,t_0}(\Omega) = S_{t_0,t}\mathcal{D}(\Omega). \tag{1.38}$$

A dynamical variable at time  $t$   $A(G_{t,t_0}(\Omega))$  can be represented in the form

$$S_{t,t_0}A(\Omega). \tag{1.38'}$$

After taking into account Equation (1.12) we have

$$S_{t_2,t_0} = S_{t_2,t_1}S_{t_1,t_0} \tag{1.39}$$

and Equation (1.15) becomes

$$S_{t,t_0} = S_{t_0,t}^{-1}, \quad S_{t_0,t} = S_{t,t_0}^{-1}. \tag{1.40}$$

We can also rewrite Equation (1.27) in the form

$$\frac{\partial \mathcal{D}_{t,t_0}}{\partial t} = -\mathcal{L}_t \mathcal{D}_{t,t_0}, \quad \mathcal{D}_{t,t_0} = \mathcal{D}_0 \quad \text{for } t = t_0, \tag{1.41}$$

where

$$\mathcal{L}_t = \sum_{1 \leq j \leq n} \left\{ \frac{\partial H(t, \Omega)}{\partial p_j} \frac{\partial}{\partial q_j} - \frac{\partial H(t, \Omega)}{\partial q_j} \frac{\partial}{\partial p_j} \right\} \tag{1.42}$$

We also note that, if we introduce the following scalar product in the space of functions

$$(f_1, f_2) = \int f_1^*(\Omega) f_2(\Omega) d\Omega$$

the operator  $\mathcal{L}_t$  is anti-Hermitian (anti-self-conjugate). Actually, integrating by parts, we get

$$\int f_1^*(\Omega) \sum_{1 \leq j \leq n} \left\{ \frac{\partial H(t, \Omega)}{\partial p_j} \frac{\partial}{\partial q_j} - \frac{\partial H(t, \Omega)}{\partial q_j} \frac{\partial}{\partial p_j} \right\} f_2(\Omega) d\Omega$$

$$\begin{aligned}
&= - \int f_2(\Omega) \sum_{1 \leq j \leq n} \left\{ \frac{\partial}{\partial q_j} \frac{\partial H(t, \Omega)}{\partial p_j} f_1^*(\Omega) - \frac{\partial}{\partial p_j} \frac{\partial H(t, \Omega)}{\partial q_j} f_1^*(\Omega) \right\} d\Omega \\
&= - \int f_2(\Omega) \{ \mathcal{L}_t f_1^*(\Omega) \} d\Omega
\end{aligned}$$

i.e.,  $(f_1, \mathcal{L}_t f_2) = -(\mathcal{L}_t f_1, f_2)$  or

$$\mathcal{L}_t^+ = -\mathcal{L}_t. \quad (1.43)$$

Therefore, Equation (1.41), which specifies the evolution of the probability density in classical mechanics, possesses some formal analogy to the wave equation of quantum mechanics

$$\frac{\partial \psi}{\partial t} = \frac{i}{\hbar} H \psi$$

where also  $(iH/\hbar)^+ = -iH/\hbar$ , and the operator  $S$  is similar to an operator characterizing the time evolution of a wave function.

Needless to say, we are speaking of a purely formal mathematical analogy, since the physical meanings of  $\psi$  and  $\mathcal{D}$  are completely different. Nevertheless, this analogy can be used to transfer certain methods of quantum mechanics to the study of the evolution of  $\mathcal{D}$  in classical systems.

We stress that such an analogy has already been noticed before.

#### 4. SYMMETRY PROPERTIES

We now discuss one more property of Equation (1.41). Let  $\Lambda$  be a linear operator which commutes with  $\mathcal{L}_t$

$$\mathcal{L}_t \Lambda = \Lambda \mathcal{L}_t. \quad (1.44)$$

If the relation

$$\Lambda \mathcal{D}_0 = \mathcal{D}_0 \quad (1.45)$$

is valid, it implies that also for any

$$\Lambda \mathcal{D}_{t, t_0} = \mathcal{D}_{t, t_0}. \quad (1.46)$$

In fact Equation (1.41) yields

$$\frac{\partial \Lambda \mathcal{D}_{t, t_0}}{\partial t} = -\mathcal{L}_t \Lambda \mathcal{D}_{t, t_0},$$

and therefore

$$\frac{\partial(\mathcal{D}_{t,t_0} - \Lambda\mathcal{D}_{t,t_0})}{\partial t} = -\mathcal{L}_t(\mathcal{D}_{t,t_0} - \Lambda\mathcal{D}_{t,t_0}).$$

On the other hand, from (1.45) we see that for  $t = t_0$

$$\mathcal{D}_{t,t_0} - \Lambda\mathcal{D}_{t,t_0} = 0$$

which implies the validity of the above statement.

Equation (1.46) can be used as a basis for derivation of symmetry properties of functions  $\mathcal{D}_{t,t_0}$ . Let us now consider the case when a dynamical system consists of  $N$  identical dimensionless particles. We put

$$\Omega = (\mathbf{q}, \mathbf{p}), \quad \mathbf{q} = (\dots, \mathbf{q}_j, \dots), \quad \mathbf{p} = (\dots, \mathbf{p}_j, \dots), \quad j = 1, \dots, N,$$

where  $\mathbf{q}_j$  and  $\mathbf{p}_j$  are three-dimensional vectors specifying the position and momentum of the  $j$ -th particle. The pair of vectors  $(\mathbf{q}_j, \mathbf{p}_j)$  thus specifies the dynamical state of the  $j$ -th particle.

Let  $P$  denote any permutation of  $N$  three-dimensional vectors. It is then clear that linear operator

$$\Lambda f(\mathbf{q}_j, \mathbf{p}_j) = f(P\mathbf{q}_j, P\mathbf{p}_j) \tag{1.47}$$

does nothing but change the numbering of the particles. Since the particles are identical, a change in their numbering cannot affect such a physical quantity as the Hamiltonian  $H(t, \mathbf{q}_j, \mathbf{p}_j)$  of the system. We therefore have

$$H(t, P\mathbf{q}_j, P\mathbf{p}_j) = H(t, \mathbf{q}_j, \mathbf{p}_j). \tag{1.48}$$

Equation (1.42) then gives

$$\mathcal{L}_t = \sum_{1 \leq j \leq n} \left\{ \frac{\partial H(t, \mathbf{q}, \mathbf{p})}{\partial \mathbf{p}_j} \frac{\partial}{\partial \mathbf{q}_j} - \frac{\partial H(t, \mathbf{q}, \mathbf{p})}{\partial \mathbf{q}_j} \frac{\partial}{\partial \mathbf{p}_j} \right\}. \tag{1.49}$$

Thus, it is obvious that, if we first change the numbering of the particles in some function  $f(\mathbf{q}, \mathbf{p})$  and then apply operator  $\mathcal{L}_t$ , we obtain the same result as if we first apply operator  $\mathcal{L}_t$  to  $f(\mathbf{q}, \mathbf{p})$  and only then change the numbering of the indices. In other words,  $\mathcal{L}_t \Lambda f(\mathbf{q}, \mathbf{p}) = \Lambda \mathcal{L}_t f(\mathbf{q}, \mathbf{p})$ , i.e., operators  $\mathcal{L}_t$  and  $\Lambda$  commute.

The above statement therefore implies that, if an initial function  $\mathcal{D}_0$  is a symmetric function of individual dynamical states of  $N$  particles

$$\mathcal{D}_0(P\mathbf{q}, P\mathbf{p}) = \mathcal{D}_0(\mathbf{q}, \mathbf{p}), \quad (1.50)$$

then  $\mathcal{D}_{t,t_0}$  at any other time  $t$  will also possess the same symmetry property

$$\mathcal{D}_{t,t_0}(P\mathbf{q}, P\mathbf{p}) = \mathcal{D}_{t,t_0}(\mathbf{q}, \mathbf{p}). \quad (1.51)$$

This property also holds in a more general case, when a dynamical system consists of particles of  $s$  types and the identity of particles takes place only within each of the types

$$\mathbf{q} = (\dots, \mathbf{q}_{j,a} \dots), \quad \mathbf{p} = (\dots, \mathbf{p}_{j,a} \dots), \\ j = 1, \dots, N, \quad q = 1, \dots, s.$$

Here  $(\mathbf{q}_{j,a}, \mathbf{p}_{j,a})$  denotes the individual dynamical state of the the  $j$ -th particle of the  $a$ -th type.

In this case, there should be invariance with respect to a change in the numbering of particles belonging to one and the same type  $a$ . Therefore, Equation (1.48) is valid only for those permutations  $P$  which act on indices  $j$  but do not change the numbers of types  $a$ . If we repeat the above speculations, we see that under such restrictions on the choice of  $P$ , the symmetry properties (1.51) will again follow from the Equation (1.48).

## 5. ISOLATED DYNAMICAL SYSTEMS

So far, we have considered the general case when a Hamiltonian  $H$  may explicitly depend on time  $t$ . We shall now consider the case when dynamical systems are totally isolated from external influence and according to Equation (1.3) the Hamiltonian does not depend explicitly on time  $t$

$$H = H(\mathbf{q}, \mathbf{p}).$$

Equations (1.42) and (1.49) then imply that linear operator  $\mathcal{L}_t$  also does not depend on  $t$

$$\mathcal{L}_t = \mathcal{L} \quad (1.52)$$

and Equations (1.41) gives

$$\frac{\partial \mathcal{D}_{t,t_0}}{\partial t} = -\mathcal{L} \mathcal{D}_{t,t_0},$$

whence

$$\mathcal{D}_{t,t_0} = e^{-(t-t_0)\mathcal{L}} \mathcal{D}_0.$$

Thus, we have  $S_{t_0,t} = e^{-(t-t_0)\mathcal{L}}$ . We see that, in this case, the evolution operator depends on  $t$  and  $t_0$  through the difference  $t - t_0$ . This is quite natural, since in the absence of an explicit dependence of the Hamiltonian  $H$  on  $t$ , the equations of motion become invariant with respect to transformations in time  $t \rightarrow t + \tau$ , so that the initial moment of time is not specific at all.

Let us take  $t_0 = 0$  as the initial time and write the evolution operator in the form

$$S_t = e^{t\mathcal{L}}. \tag{1.53}$$

Then we have

$$\mathcal{D}_t = S_{-t}\mathcal{D}_0 = e^{-t\mathcal{L}} \mathcal{D}_0. \tag{1.54}$$

Similarly, a dynamical variable at time  $t$   $A(\Omega(t)) = A_t(\Omega)$  can be represented in the form

$$A_t(\Omega) = S_t A(\Omega) = e^{-t\mathcal{L}} A(\Omega). \tag{1.55}$$

Hence, it follows that

$$\frac{\partial A_t}{\partial t} = \mathcal{L} A_t \tag{1.56}$$

or, taking into consideration form (1.42) and (1.49) of operator  $\mathcal{L}$ , we obtain

$$\frac{\partial A_t}{\partial t} = [A_t, H]. \tag{1.57}$$

Therefore, Equation (1.33) gives

$$\langle A_t \rangle = \int A_t(\Omega) \mathcal{D}(\Omega) d\Omega = \int A(\Omega) \mathcal{D}_t(\Omega) d\Omega. \tag{1.58}$$

## 6. A SYSTEM OF IDENTICAL MONOATOMIC MOLECULES

As an example, we shall consider a dynamical system of  $N$  identical monoatomic molecules. The usual model for such a system is that of  $N$  material points with kinetic energy

$$\frac{1}{2m} \sum_{1 \leq j \leq N} \mathbf{p}_j^2 \tag{1.59}$$

and potential energy of binary interactions

$$\sum_{1 \leq j_1 < j_2 \leq N} \Phi(\mathbf{q}_{j_1} - \mathbf{q}_{j_2}), \quad \Phi(\mathbf{q}) = \Phi(-\mathbf{q}) \quad (1.59')$$

where  $\Phi(\mathbf{q}) = \Phi(|\mathbf{q}|)$  is a spherical symmetric function describing the interaction of a pair of particles.

In order to take into account the fact that the particles of a given dynamical system should be confined to some finite value  $V$ , a so called potential barrier may be introduced. Let us introduce a potential  $U(\mathbf{q})$ , which is equal to zero within  $V$ , except for a narrow boundary region, and rapidly tends to infinity  $U(\mathbf{q}) \rightarrow \infty$  when  $\mathbf{q}$  approaches the boundary of  $V$ .

Then, if we add the term

$$\sum_{1 \leq j \leq N} U(\mathbf{q}_j) \quad (1.60)$$

to the Hamiltonian, it is guaranteed that particle within volume  $V$  will not leave it. Moreover, the motion of particles within  $V$ , except for narrow boundary region mentioned above, is described by a Hamiltonian which is the sum of the kinetic energy (1.59) and the potential energy (1.59') only.

Taking the additional potential energy (1.60) into account, we write the total Hamiltonian of the system in the form

$$H = \sum_{1 \leq j \leq N} \left\{ \frac{\mathbf{p}_j^2}{2m} + U(\mathbf{q}_j) \right\} + \sum_{1 \leq j_1 < j_2 \leq N} \Phi(\mathbf{q}_{j_1} - \mathbf{q}_{j_2}) \quad (1.61)$$

and therefore

$$\begin{aligned} \mathcal{L} = \sum_{1 \leq j \leq N} \left\{ \frac{\mathbf{p}_j}{m} \frac{\partial}{\partial \mathbf{q}_j} - \frac{\partial U(\mathbf{q}_j)}{\partial \mathbf{q}_j} \frac{\partial}{\partial \mathbf{p}_j} \right\} \\ + \sum_{1 \leq j_1 < j_2 \leq N} \frac{\partial}{\partial \mathbf{q}_{j_1}} \Phi(\mathbf{q}_{j_1} - \mathbf{q}_{j_2}) \left\{ \frac{\partial}{\partial \mathbf{p}_{j_2}} - \frac{\partial}{\partial \mathbf{p}_{j_1}} \right\}. \quad (1.62) \end{aligned}$$

It is clear that such a Hamiltonian (1.61) is invariant with respect to change of sign of all momenta

$$H(\mathbf{q}, \mathbf{p}) = H(\mathbf{q}, -\mathbf{p}). \quad (1.63)$$

## 7. PROPERTY OF REVERSIBILITY

We now show that for a dynamical system whose Hamiltonian satisfies condition (1.63), the so called property of reversibility holds. In fact, Equation (1.63) implies

$$\mathcal{L}f(\mathbf{q}, -\mathbf{p}) = -\{\mathcal{L}f(\mathbf{q}, \mathbf{p})\}_{\mathbf{p} \rightarrow -\mathbf{p}}.$$

Therefore, if we perform the transformation in Equation (1.54)  $\mathbf{p} \rightarrow -\mathbf{p}$ ,  $t \rightarrow -t$ , we find

$$\mathcal{D}_{-t}(\mathbf{q}, -\mathbf{p}) = e^{-t\mathcal{L}} \mathcal{D}_0(\mathbf{q}, \mathbf{p}). \quad (1.64)$$

Consequently, if  $\mathcal{D}_t(\mathbf{q}, \mathbf{p})$  is a solution of the Liouville equation

$$\frac{\partial \mathcal{D}_t}{\partial t} = -\mathcal{L}\mathcal{D}_t,$$

then, by inverting the sign of all momenta and time  $\mathcal{D}_{-t}(\mathbf{q}, -\mathbf{p})$  we again obtain a solution of the same equation. This is just the so called property of reversibility.

Of course, individual motions in phase space also possess the property of reversibility. In fact, the Hamiltonian equations show that, if  $\Omega(t) = \{\mathbf{q}(t), \mathbf{p}(t)\}$  is a solution of these equations, then the reversed equation  $\bar{\Omega}(t) = \{\mathbf{q}(-t), -\mathbf{p}(-t)\}$  also satisfies the Hamiltonian equations.