Noname manuscript No.
(will be inserted by the editor)

On the Gibbs-Liouville theorem in classical mechanics

Andreas Henriksson

Received: date / Accepted: date

Abstract In this article, it is argued that the Gibbs-Liouville theorem is a mathematical representation of the statement that closed classical systems evolve deterministically. From the perspective of an observer of the system, whose knowledge about the degrees of freedom of the system is complete, the statement of deterministic evolution is equivalent to the notion that the physical distinctions between the possible states of the system, or, in other words, the information possessed by the observer about the system, is never lost. Thus, it is proposed that the Gibbs-Liouville theorem is a statement about the dynamical evolution of a closed classical system valid in such situations where information about the system is conserved in time. Furthermore, in this article it is shown that the Hamilton equations and the Hamilton principle on phase space follow directly from the differential representation of the Gibbs-Liouville theorem, i.e. that the divergence of the Hamiltonian phase flow velocity vanish. Thus, considering that the Lagrangian and Hamiltonian formulations of classical mechanics are related via the Legendre transformation, it is obtained that these two standard formulations are both logical consequences of the statement of deterministic evolution, or, equivalently, information conservation.

Keywords Determinism · Information · Gibbs-Liouville theorem · Hamilton equations · Hamilton principle

PACS 45.20.Jj · 45.05.+x · 45.20.-d · 03.50.-z

Andreas Henriksson
St.Olav school, Jens Zetlitzgt. 33, 4008, Stavanger; Norway
E-mail: andreas.henriksson@skole.rogfk.no
ORCID: 0000-0001-9014-4320

Contents

1 Introduction

A key concept which is at the heart of the distinction between the temporal evolution of classical and quantum systems is determinism. Classical systems are said to be deterministic while quantum systems are non-deterministic. Considering this key distinction, it is the purpose of this article to initiate a study on the role of determinism in classical and quantum mechanics by rephrasing the conventional exposition of classical mechanics in such a manner that the notion of deterministic evolution take the central role.

The conventional exposition of classical mechanics is largely based on the historical development of the subject [1][2][3][4]. Newton introduced the concept of force in order to describe the motion of objects, as mathematically expressed by his second law of motion, which is a second-order differential equation in time. Later, Lagrange [5][6] constructed a mathematically equivalent formulation where the Lagrangian function, which is defined on configuration space, is introduced and which play the central role. The Lagrange, or Euler-Lagrange, equations of motion are also second-order differential equations in time. Lagrange's formulation was later transformed from configuration space onto phase space by Hamilton [7], where the central role is played by the Hamiltonian function. The Hamilton equations of motion are first-order differential equations in time. The deterministic character must then be proved by showing that the equations of motion, with known unique initial conditions, have unique solutions such that the states cannot converge into each other. Thus, determinism enter into the discussion at a fairly late stage, after the introduction and definition of concepts such as force, the Lagrangian and Hamiltonian functions, and after the equations of motion have been obtained. In this article, the attempt is to start with the notion of determinism and from it deduce the necessary form of the equations of motion.

The purpose behind the desire to shift the exposition of classical mechanics as proposed in this article is to, hopefully, better understand the non-deterministic evolution for quantum systems on phase space, as described in the seminal paper by Moyal [8].

2 Phase space

The theatrical stage on which physical phenomena are played out are characterized by so-called degrees of freedom. They are parameters whose values are aimed at defining the state of existence for a system as it unfold in time. There exist different mathematical representations of this theatrical stage. In this article, the space of phases, or phase space, is the stage used to study the flow of classical systems.

At any given time t, any given particle j within an $N-$particle system with three spatial dimensions has the spatial location $\mathbf{q}_j \equiv (q_1, q_2, q_3)_j$ and the momenta $\mathbf{p}_j \equiv (p_1, p_2, p_3)_j$. These are the degrees of freedom for the j'th particle. The total number of degrees of freedom for the system is thus $6N$. For notational simplicity, the $3N$ spatial and the $3N$ momenta degrees of freedom are denoted by q and p, respectively. The space of all possible values for the pair (q, p) define the phase space. Each point in phase space correspond to a specific state for the system, i.e. a specific value for the spatial location and momenta of each particle within the system.

For continuous systems, all states in which the system can exist are continuously connected to each other in the sense that any two arbitrary states can be transformed into each other by considering successive infinitesimal variations in q and p. Thus, in the continuous case, the states of a system lie on smooth surfaces in phase space, see figure 1, where the state at time t_0, given by the values (q_0, p_0), is connected to the state at another time t, given by the values $(q(t), p(t))$, along a smooth trajectory, the so-called system trajectory. Phase space can be extended to explicitly include time as a coordinate which is orthogonal to phase space, see figure 2. As the system evolve in time, it traces out a trajectory in the extended phase space. If the trajectory on phase space is known for a given system, it mean that the entire evolutionary history of the system is known.

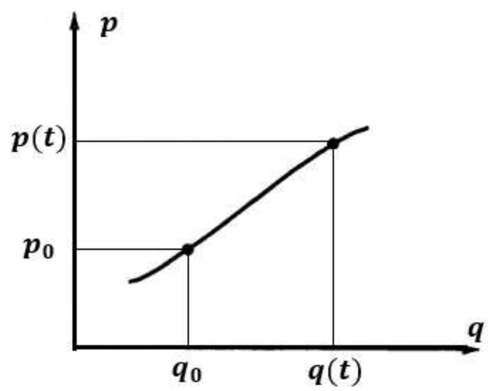

Fig. 1 Phase space for a continuous system.

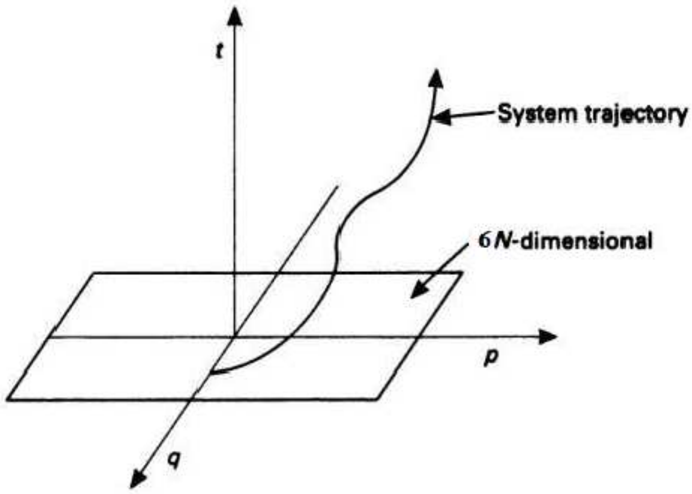

Fig. 2 The extended phase space.

3 Determinism and information

In classical mechanics, it is a fundamental assumption that the evolution of a system is deterministic in both directions of time, i.e. both into the future and into the past. Deterministic evolution of a system mean that it is possible, with absolute certainty, to say that any given state of the system evolved from a definite single state in the past and will evolve into a definite single state in the future. There cannot be any ambiguity in the evolutionary history of a system. Thus, deterministic evolution imply that nowhere on phase space can states converge or diverge, see figure 3.

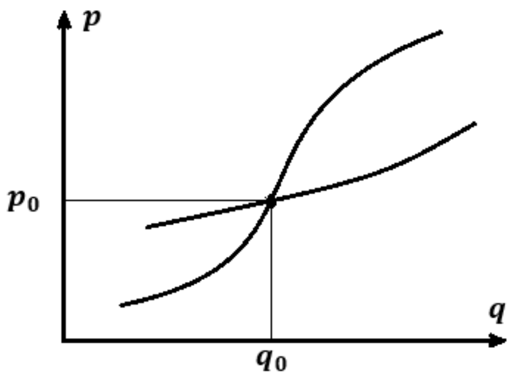

Fig. 3 Non-deterministic evolution imply that system trajectories would cross each other on phase space, here at point (q_0, p_0).

Systems that appear to evolve non-deterministically give rise to the appearance of irreversible processes in nature. The reason for this is that if a system start out in a given state it is not necessarily the case that the system end up at the same initial state by reversing the motion of the system in time. An example of a seemingly irreversible process is the sliding of a block of cheese along a table. Due to friction the block will always come to rest, apparently independent on the initial condition of the block. Thus it appear as though the multitude of possible initial states for the block, given by the possibility of sending off the block with different initial speeds, all converge to the same final state where the block is at rest. Knowing the final state of the system does not help in predicting the initial state of the system. Therefore, the experiment with sending off the block of cheese seem to represent an evolution which is non-deterministic into the past.

The origin for the apparent violation of reversibility in physical processes is not due to a fundamental character in physical laws, but rather it is due to the ignorance of the observer. The observer has not taken into account all the details of the system. Degrees of freedom for the system has been ignored. In the case of the sliding block of cheese, it is the individual motion of atoms in the block and table which has been ignored. Assuming that all degrees of freedom for the block and table are followed in perfect detail as the block slide on the table it is clear that each unique initial state will give rise to a unique final state where the distinction between the final states are given by the distinct final position and velocity of each atom in the block and table.

A direct consequence of the assumption of deterministic evolution is that distinctions between physical states never disappear. If there is an initial distinction between states, this distinction will survive throughout the entire motion of the system. That distinctions between states seem to disappear as time unfold is merely a consequence of the difficulty for an observer to keep perfect track of the motion of all particles. In the case of the sliding block, for a human observer, the distinction between individual motions of atoms in the block and table are too small to measure and therefore it appear as though two distinct initial states, characterized by distinct initial speeds, which are easy to measure, converge to the same final state, i.e. that the block is at rest. In conclusion, the assumption of deterministic evolution can equivalently be stated as follows.

The distinction between physical states of a closed system is conserved in time.

Due to the conservation of distinction between physical states, any set of states which lie in the interior of some volume element on phase space will remain interior of this volume element as the system evolve in time.

If a system is followed, as it evolve in time, in perfect detail by an observer, it mean that the observer has perfect and complete knowledge about all the degrees of freedom of the system, i.e. the observer know, with infinite precision, the exact position and momenta of all particles within the system. In such an ideal scenario, the observer has no problem to see the distinction between states of the system. The amount of knowledge, or information, about the system possessed by the observer, at any instant of time, is complete. Since the ideal observer never loose track of the system, the distinction between states is never lost. In other words, the knowledge, or information, that the observer has about the system is not lost as the system evolve in time.

If, however, as is the case in practical reality, the observer has a limited ability to track the motion of individual particles, the observer do not possess complete information about the system. Even worse, the observer may, as is usually the case for complicated systems with many degrees of freedom, find it more and more difficult to track the system as time unfold. In such a scenario, the amount of information about the system, possessed by the observer, decrease with time. In other words, from the perspective of the ignorant observer, information about the system is lost. However, it is important to emphasize that this apparent loss of information is entirely due to the ignorance of the observer. If all the degrees of freedom were tracked with infinite precision, information would never be lost. In the case of the sliding block of cheese, the observer has lost information because the system was known to exist in one of two distinct initial states, obtained by measuring the initial speed of the block, whereas it is not possible to distinguish between the two final states.

In conclusion, the loss of distinction between states imply that information has been lost. Thus, the conservation of distinction between states can equivalently be stated as an assumption of information conservation:

The information contained within a closed system is conserved in time.

In other words, the assumption that classical systems evolve deterministically, i.e. that the state of the system is perfectly predictable by an observer both into the future and back to the past, is equivalent to the statement that an observer of the system possess complete information about the system, and assuming that the system is closed, this amount of information is never lost.

4 Incompressible fluid flow

To understand how the statement of deterministic evolution, or, equivalently, information conservation, can be represented mathematically, consider first, as an analog, the incompressible fluid flow of identical molecules in one and two spatial dimensions.

For a fluid flow in one spatial dimension x, see figure 4, where the fluid molecules are represented as dots, the velocity v of the flow is determined by the number of molecules N that pass through a given location along x during a given time interval Δt. The rate of flow of

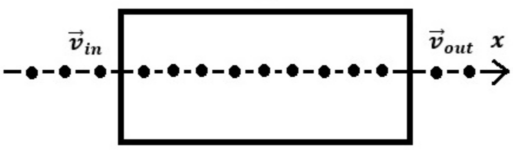

Fig. 4 Fluid flow in one spatial dimension.

the fluid, per time interval Δt, is given by

$$rate\ of\ flow = \rho(x)v(x) \tag{1}$$

where $\rho(x)$ is the density of molecules along x. In order to avoid an increase or decrease in the number of molecules within a region Δx during an instant of time Δt, i.e.

$$\frac{\Delta N}{\Delta t} = 0 \tag{2}$$

the necessary condition is that the incoming and outgoing flows are equal, i.e.

$$\rho(x_{out})v(x_{out}) = \rho(x_{in})v(x_{in}) \tag{3}$$

This is rewritten as

$$\Delta\left(\rho(x)v(x)\right) \equiv \rho(x_{out})v(x_{out}) - \rho(x_{in})v(x_{in}) = 0 \tag{4}$$

In differential form it read

$$d\left(\rho(x)v(x)\right) \equiv \frac{d}{dx}\left(\rho(x)v(x)\right) \cdot \Delta x = 0 \tag{5}$$

which gives that

$$\frac{d}{dx}\left(\rho(x)v(x)\right) = 0 \tag{6}$$

For the number of molecules to be conserved over an extended period of time, i.e. over many successive time intervals Δt, the required condition become

$$\frac{\partial\rho(x,t)}{\partial t} + \frac{\partial}{\partial x}\left(\rho(x,t)v(x)\right) = 0 \tag{7}$$

This is the continuity equation for the flow of molecules in one dimension. The product rule on the second term give

$$\frac{\partial\rho(x,t)}{\partial t} + \frac{\partial\rho(x,t)}{\partial x} \cdot v(x) + \rho(x,t) \cdot \frac{\partial v(x)}{\partial x} = 0 \tag{8}$$

where the first two terms are equal to the total time derivative of the density, i.e.

$$\frac{d\rho(x,t)}{dt} = \frac{\partial\rho(x,t)}{\partial t} + \frac{\partial\rho(x,t)}{\partial x} \cdot \frac{\partial x}{\partial t} \tag{9}$$

The continuity equation can thus be rewritten as

$$\frac{d\rho(x,t)}{dt} + \rho(x,t) \cdot \frac{\partial v(x)}{\partial x} = 0 \tag{10}$$

Thus, if the velocity of the flow is independent on x, i.e. if

$$\frac{\partial v(x)}{\partial x} = 0 \tag{11}$$

then the density of molecules is constant in time as the fluid flow along x, i.e.

$$\frac{d\rho(x,t)}{dt} = 0 \tag{12}$$

Such a flow is referred to as an incompressible flow because the condition that the density of molecules at any given location x within Δx do not change over time ensure that the molecules do not lump together. Thus, in conclusion, a necessary and sufficient condition for the one-dimensional fluid to be incompressible is that the divergence of the flow velocity vanish, i.e. that $\frac{\partial v(x)}{\partial x} = 0$.

Consider now the flow of a fluid in two spatial dimensions, x and y, see figure 5. If the number of molecules

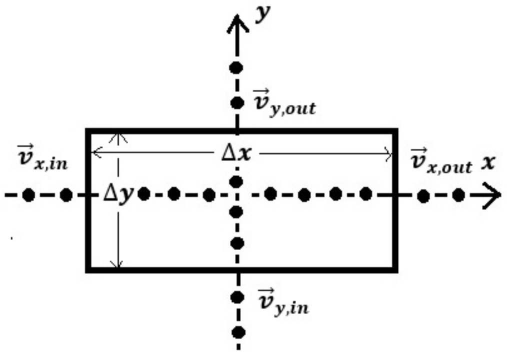

Fig. 5 Fluid flow in two spatial dimensions.

within the fixed area $\varDelta x \cdot \varDelta y$ within any given time interval $\varDelta t$ is to stay constant, the necessary condition relating the incoming and outgoing flows is given by

$$\varDelta \left(\rho(x,y)v_x(x,y)\right) + \varDelta \left(\rho(x,y)v_y(x,y)\right) = 0 \tag{13}$$

where $\varDelta \left(\rho(x,y)v_x(x,y)\right)$ and $\varDelta \left(\rho(x,y)v_y(x,y)\right)$ are defined by, respectively,

$$\{\rho(x_{out},y)v_x(x_{out},y) - \rho(x_{in},y)v_x(x_{in},y)\} \cdot \varDelta y \tag{14}$$

and

$$\{\rho(x,y_{out})v_y(x,y_{out}) - \rho(x,y_{in})v_y(x,y_{in})\} \cdot \varDelta x \tag{15}$$

In differential form, they read

$$d\left(\rho(x,y)v_x(x,y)\right) = \frac{\partial}{\partial x}\left(\rho(x,y)v_x(x,y)\right)\varDelta x \varDelta y \tag{16}$$

$$d\left(\rho(x,y)v_y(x,y)\right) = \frac{\partial}{\partial y}\left(\rho(x,y)v_y(x,y)\right)\varDelta y \varDelta x \tag{17}$$

Thus, the condition become

$$\frac{\partial}{\partial x}\left(\rho(x,y)v_x(x,y)\right) + \frac{\partial}{\partial y}\left(\rho(x,y)v_y(x,y)\right) = 0 \tag{18}$$

For the number of molecules to be constant over an arbitrary length of time, the necessary condition take the form, dropping spacetime coordinates in the notation for convenience,

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}\left(\rho v_x\right) + \frac{\partial}{\partial y}\left(\rho v_y\right) = 0 \tag{19}$$

This is the continuity equation for the flow of molecules in two dimensions. Using the product rule and noting that the total time derivative of the density is given by

$$\frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial x} \cdot v_x + \frac{\partial \rho}{\partial y} \cdot v_y \tag{20}$$

the continuity equation can be rewritten as

$$\frac{d\rho}{dt} + \rho \cdot \left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y}\right) = 0 \tag{21}$$

or, in vector notation,

$$\frac{d\rho}{dt} + \rho \boldsymbol{\nabla} \cdot \mathbf{v} = 0 \tag{22}$$

Thus, if the divergence of the flow velocity vanish, i.e. if

$$\boldsymbol{\nabla} \cdot \mathbf{v} = 0 \tag{23}$$

then the density of molecules is constant in time as the fluid flow in x and y, i.e.

$$\frac{d\rho}{dt} = 0 \tag{24}$$

A necessary and sufficient condition that the fluid flow is incompressible is thus that the divergence of the flow velocity vanish.

5 The Gibbs-Liouville theorem

Consider an arbitrary region $\varOmega$ on phase space, with volume $V_{\varOmega}$ and volume element $\varDelta q \varDelta p$, see figure 6. In

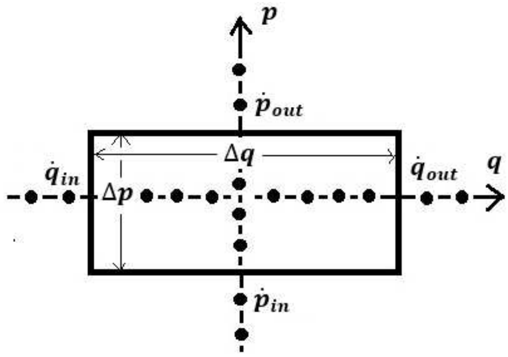

Fig. 6 Hamiltonian flow on phase space.

order for the number of states N within the phase space volume $\varOmega$ to neither increase nor decrease within the time interval $\varDelta t$, i.e.

$$\frac{\varDelta N}{\varDelta t} = 0 \tag{25}$$

it is necessary that the incoming and outgoing flows cancel, i.e. that

$$\varDelta \left(\rho(q,p)\dot{q}\right) + \varDelta \left(\rho(q,p)\dot{p}\right) = 0 \tag{26}$$

where $\rho(q,p)$ is the density of states on phase space, and the flow differences are defined by, respectively,

$$\varDelta \left(\rho(q,p)\dot{q}\right) \equiv \{\rho(q_{out},p))\dot{q}_{out} - \rho(q_{in},p))\dot{q}_{in}\}\, \varDelta p \tag{27}$$

and

$$\varDelta \left(\rho(q,p)\dot{p}\right) \equiv \{\rho(q,p_{out}))\dot{p}_{out} - \rho(q,p_{in}))\dot{p}_{in}\}\, \varDelta q \tag{28}$$

In differential form the condition 25 read

$$\frac{\partial}{\partial q}\left(\rho(q,p)\dot{q}\right) + \frac{\partial}{\partial p}\left(\rho(q,p)\dot{p}\right) = 0 \tag{29}$$

where

$$d\left(\rho(q,p)\dot{q}\right) = \frac{\partial}{\partial q}\left(\rho(q,p)\dot{q}\right) \mathit{\Delta} q \mathit{\Delta} p \tag{30}$$

$$d\left(\rho(q,p)\dot{p}\right) = \frac{\partial}{\partial p}\left(\rho(q,p)\dot{p}\right) \mathit{\Delta} p \mathit{\Delta} q \tag{31}$$

Extending the condition 25 to be valid for an arbitrary length of time, the differential condition 29 become, dropping reference to the phase space degrees of freedom in the arguments of the density function for convenience,

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial q}\left(\rho \dot{q}\right) + \frac{\partial}{\partial p}\left(\rho \dot{p}\right) = 0 \tag{32}$$

or, in vector notation,

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \mathbf{v}) = 0 \tag{33}$$

where

$$\boldsymbol{\nabla} \equiv \left(\frac{\partial}{\partial q}, \frac{\partial}{\partial p}\right) \tag{34}$$

is the differential operator on phase space, and

$$\mathbf{v} \equiv (\dot{q}, \dot{p}) \tag{35}$$

is the velocity by which states flow on phase space. The continuity equation 33 is the Gibbs-Liouville equation [9][10] for the density of states on phase space. It say that the number of states is locally conserved. The term $\boldsymbol{\nabla} \cdot (\rho \mathbf{v})$ represent the net flow of states through $\mathit{\Omega}$, i.e. the difference between the outflow and inflow of states. The continuity equation thus state that if there is a net outflow of states, i.e. if

$$\boldsymbol{\nabla} \cdot (\rho \mathbf{v}) > 0 \tag{36}$$

then the density of states within $\mathit{\Omega}$ decrease with time, i.e.

$$\frac{\partial \rho}{\partial t} = -\boldsymbol{\nabla} \cdot (\rho \mathbf{v}) < 0 \tag{37}$$

If there is a net inflow of states, i.e. if

$$\boldsymbol{\nabla} \cdot (\rho \mathbf{v}) < 0 \tag{38}$$

then the density of states within $\mathit{\Omega}$ increase with time, i.e.

$$\frac{\partial \rho}{\partial t} = -\boldsymbol{\nabla} \cdot (\rho \mathbf{v}) > 0 \tag{39}$$

Using that the total time derivative of the density of states is given by

$$\begin{aligned} \frac{d\rho}{dt} &= \frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial q}\dot{q} + \frac{\partial \rho}{\partial p}\dot{p} &(40)\\ &= \frac{\partial \rho}{\partial t} + (\boldsymbol{\nabla}\rho) \cdot \mathbf{v} &(41)\end{aligned}$$

and the product rule

$$\boldsymbol{\nabla} \cdot (\rho \mathbf{v}) = (\boldsymbol{\nabla}\rho) \cdot \mathbf{v} + \rho \boldsymbol{\nabla} \cdot \mathbf{v} \tag{42}$$

the continuity equation can be rewritten as

$$\frac{d\rho}{dt} + \rho\ \boldsymbol{\nabla} \cdot \mathbf{v} = 0 \tag{43}$$

Thus, if the divergence of the phase flow velocity vanish, i.e. if

$$\boldsymbol{\nabla} \cdot \mathbf{v} = 0 \tag{44}$$

then, by the continuity equation, the density of states on phase space is constant in time along the flow on phase space, i.e.

$$\frac{d\rho}{dt} = 0 \tag{45}$$

In such a situation, the flow of the system on phase space is incompressible because the condition that the density of states at any given location (q,p) on phase space, within an arbitrary region $\mathit{\Omega}$, do not change over time ensure that the states do not lump together. In other words, in conclusion, a necessary and sufficient condition for the flow of the system on phase space to evolve deterministically, or, equivalently, to conserve information, is that the divergence of the phase flow velocity vanish. This conclusion is referred to as the Gibbs-Liouville theorem [9][10].

The Gibbs-Liouville continuity equation can be derived more shortly by considering the relation between the number of states N and the density of states $\rho(q,p,t)$, i.e.

$$N = \int_{V_{\mathit{\Omega}}} \rho(q,p,t)\, dq dp \tag{46}$$

Thus,

$$\begin{aligned} \frac{dN}{dt} &= \frac{d}{dt}\int_{V_{\mathit{\Omega}}} \rho(q,p,t)\, dq dp \\ &= \int_{V_{\mathit{\Omega}}} \left(\frac{d\rho}{dt} + \rho\ \boldsymbol{\nabla} \cdot \mathbf{v}\right) dq dp \\ &= 0 &(47)\end{aligned}$$

Since information should be conserved independently on the size of $\mathit{\Omega}$, the integrand in equation 47 must vanish for arbitrary volumes $V_{\mathit{\Omega}}$, giving the desired result

$$\frac{d\rho}{dt} + \rho\ \boldsymbol{\nabla} \cdot \mathbf{v} = 0 \tag{48}$$

6 Hamilton's equations

The vanishing divergence of the flow velocity, written out explicitly in terms of the velocity components $\dot{q}$ and $\dot{p}$, become

$$\frac{\partial \dot{q}}{\partial q} + \frac{\partial \dot{p}}{\partial p} = 0 \tag{49}$$

For this condition to hold, the velocity components must both be related to a function $\mathcal{H}(q,p)$ on phase space given by the Hamilton equations, i.e.

$$\dot{q} = \frac{\partial \mathcal{H}}{\partial p} \tag{50}$$

$$\dot{p} = -\frac{\partial \mathcal{H}}{\partial q} \tag{51}$$

Thus, given the function $\mathcal{H}(q,p)$, the flow of the system in time is determined by how $\mathcal{H}(q,p)$ change on phase space. In this sense, $\mathcal{H}(q,p)$ is said to be the generator for the motion in time of the system. The flow of the system on phase space is then referred to as a Hamiltonian flow.

7 The Hamiltonian and Lagrangian

The Hamilton equation 50 correspond to the integral equation

$$\mathcal{H}(p) = \int dp\ \dot{q}(p) \tag{52}$$

The momentum p and speed $\dot{q}$ are assumed to be in one-to-one correspondence. This mean that for each value of $\dot{q}$ there is a unique value for p, and vice versa. The function $\mathcal{H}(p)$ is then geometrically interpreted as the unique area under the $\dot{q}(p)-$graph, bounded by $(0,p)$ and $(0,\dot{q}(p))$, see figure 7. Due to the one-to-one correspondence between p and $\dot{q}$ it is possible to define a related area, $\mathcal{L}(\dot{q})$, given by the unique area under the $p(\dot{q})-$graph,

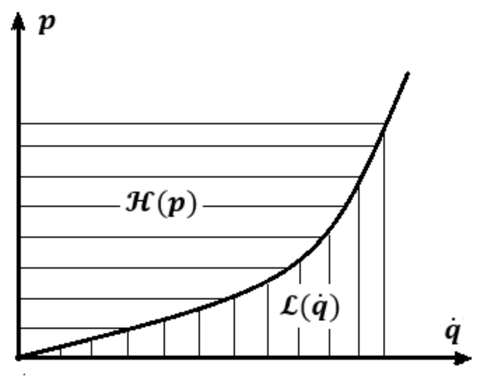

Fig. 7 The areas under $\dot{q}(p)$ and $\dot{p}(q)$ graphs define the Hamiltonian and Lagrangian, respectively.

$$\mathcal{L}(\dot{q}) = \int d\dot{q}\ p(\dot{q}) \tag{53}$$

This integral equation correspond to the differential equation[1]

$$\frac{d\mathcal{L}(\dot{q})}{d\dot{q}} = p \tag{54}$$

The total area of the rectangle bounded by $(0,p)$ and $(0,\dot{q})$ is given by

$$\mathcal{L}(\dot{q}) + \mathcal{H}(p) = p \cdot \dot{q} \tag{55}$$

It is possible to include a dependence on the generalized coordinate q under the constraint that any $q-$dependent terms in the functions $\mathcal{H}$ and $\mathcal{L}$ cancel such that the total area is $q-$independent. Thus, in general, the functions $\mathcal{H}$ and $\mathcal{L}$, referred to as the Hamiltonian and the Lagrangian, respectively, satisfy the so-called Legendre transformation,

$$\mathcal{L}(q,\dot{q}) + \mathcal{H}(q,p) = p \cdot \dot{q} \tag{56}$$

where

$$\mathcal{L}(q,\dot{q}) = \int_0^{\dot{q}} d\dot{q}\ p(\dot{q}) - U(q) \tag{57}$$

$$\mathcal{H}(q,p) = \int_0^{p} dp\ \dot{q}(p) + U(q) \tag{58}$$

The function $U(q)$ is referred to as the potential energy of the system. The requirement that the total area is $q-$independent cause the Lagrangian and Hamiltonian to have a relative sign difference for their potential energy.

8 Principle of stationary action

The Hamilton equations

$$-\frac{\partial \mathcal{H}}{\partial q} - \dot{p} = 0 \tag{59}$$

$$\dot{q} - \frac{\partial \mathcal{H}}{\partial p} = 0 \tag{60}$$

is the local, differential, representation of the principle of information conservation on phase space. A global, or integral, representation can be obtained by considering the entire evolutionary path from some initial time t_i to some final time t_f where the Hamilton equations are integrated over time[2]. For this purpose, multiply the Hamilton equations with two independent arbitrary

[1] In the Lagrangian formulation of classical mechanics, this differential equation is the defining equation for the momenta conjugate to the generalized coordinate.

[2] For the derivation of an integral representation on configuration space starting from Newton's second law of motion, see chapter 10 in reference [11].

functions of time, $\delta q(t)$ and $\delta p(t)$, representing, respectively, small displacements in q and p on phase space, in the following manner,

$$\left(-\frac{\partial \mathcal{H}}{\partial q} - \dot{p}\right)\delta q(t) = 0 \quad (61)$$

$$\left(\dot{q} - \frac{\partial \mathcal{H}}{\partial p}\right)\delta p(t) = 0 \quad (62)$$

The displacements $\delta q(t)$ and $\delta p(t)$ are pictured as slight variations of the physical path on phase space, i.e.

$$q(t) \to q(t) + \delta q(t) \quad (63)$$

$$p(t) \to p(t) + \delta p(t) \quad (64)$$

Equations 61 and 62 are equivalent to the Hamilton equations since they hold for arbitrary variations. The fact that it is necessary to introduce two displacement functions is due to the independence of the state parameters q and p. The boundary conditions are given by

$$\delta q(t_i) = \delta q(t_f) = 0 \quad (65)$$

$$\delta p(t_i) = \delta p(t_f) = 0 \quad (66)$$

i.e. the variations vanish at the initial and final times. Integrating the Hamilton equations over time from t_i to t_f give, to leading order in the variations,

$$\int_{t_i}^{t_f} dt \left[\left(-\frac{\partial \mathcal{H}}{\partial q} - \dot{p}\right)\delta q(t) + \left(\dot{q} - \frac{\partial \mathcal{H}}{\partial p}\right)\delta p(t)\right] = 0 \quad (67)$$

Integration by parts and recalling the boundary conditions give

$$\begin{aligned} 0 &= \int_{t_i}^{t_f} dt \left[\frac{\partial(\dot{q}p - \mathcal{H})}{\partial q} - \frac{d}{dt}\frac{\partial(\dot{q}p - \mathcal{H})}{\partial \dot{q}}\right]\delta q(t) \\ &+ \int_{t_i}^{t_f} dt \left[\frac{\partial(\dot{q}p - \mathcal{H})}{\partial p} - \frac{d}{dt}\frac{\partial(\dot{q}p - \mathcal{H})}{\partial \dot{p}}\right]\delta p(t) \\ &= \int_{t_i}^{t_f} dt\ \delta\left(\dot{q}p - \mathcal{H}\right) \\ &= \delta \int_{t_i}^{t_f} dt\ \left(\dot{q}p - \mathcal{H}\right) \\ &= \delta \int_{t_i}^{t_f} dt\ \mathcal{L} \\ &= \delta \mathcal{A} \end{aligned} \quad (68)$$

where

$$\mathcal{A} \equiv \int_{t_i}^{t_f} dt\ \mathcal{L} \quad (69)$$

is the action of the system. This is Hamilton's formulation of the principle of stationary action, or shortly, Hamilton's principle. It is a global representation of information conservation, i.e. a statement on the entire evolutionary path which must be satisfied if the system is to adhere to the principle of information conservation.

Since the Hamilton principle can be derived from the Hamilton equations, which in turn is an immediate consequence of the requirement that the divergence of the Hamiltonian flow velocity vanish, it should be possible to obtain the Hamilton principle directly from the requirement that $\boldsymbol{\nabla} \cdot \mathbf{v} = 0$ is invariant under the displacements $\delta q(t)$ and $\delta p(t)$. Given that the variations are small, the flow velocity $\mathbf{v}$ can be expanded as a Taylor series about the state (q, p) where terms that are of quadratic, or higher, order in the variations δq and δp can be ignored. The infinitesimal change in $\mathbf{v}$ thus become

$$\delta \mathbf{v} = \mathbf{v}(q + \delta q, p + \delta p) - \mathbf{v}(q, p) = \delta q \frac{\partial}{\partial q}\mathbf{v} + \delta p \frac{\partial}{\partial p}\mathbf{v} \quad (70)$$

The divergence of the flow velocity transform as

$$\boldsymbol{\nabla} \cdot \mathbf{v} \to \boldsymbol{\nabla} \cdot (\mathbf{v} + \delta \mathbf{v}) = \boldsymbol{\nabla} \cdot \mathbf{v} + \boldsymbol{\nabla} \cdot \delta \mathbf{v} \quad (71)$$

If $\boldsymbol{\nabla} \cdot \delta \mathbf{v} \neq 0$, information is not conserved for the deviated path. Therefore, it is required that

$$\boldsymbol{\nabla} \cdot \delta \mathbf{v} = 0 \quad (72)$$

which is equivalent to

$$\delta\left(\boldsymbol{\nabla} \cdot \mathbf{v}\right) = 0 \quad (73)$$

This statement is for a blob of volume dV which enclose the single state (q, p). Information conservation should hold for all varied states along the evolutionary path of the system, from the initial state (q_i, p_i), at time t_i, to the final state (q_f, p_f), at time t_f. Thus, the above statement should be integrated over all blobs of volume dV along the path, i.e. the integration is over a tube, with volume V, whose interior define the region of extended phase space where the principle of information conservation is fulfilled. Thus,

$$\delta \int_{t_i}^{t_f} dt \int_V dV\ \boldsymbol{\nabla} \cdot \mathbf{v} = 0 \quad (74)$$

Applying the divergence theorem

$$\int_V dV\ \boldsymbol{\nabla} \cdot \mathbf{v} = \int_{\partial V} \mathbf{dS} \cdot \mathbf{v} \quad (75)$$

give

$$\delta \int_{t_i}^{t_f} dt \int_{\partial V} \mathbf{dS} \cdot \mathbf{v} = 0 \quad (76)$$

The integrand $\mathbf{dS} \cdot \mathbf{v}$ represent the density of the net Hamiltonian flow out of the tube. The surface area element $\mathbf{dS}$ is given by

$$\mathbf{dS} = dS\ \mathbf{n} \quad (77)$$

where $\mathbf{n} = (p, q)$ is the normal vector to the surface of the tube, i.e. $\mathbf{n}$ give the direction in phase space in which the system has to flow if it is to eventually reach a region where the principle of conservation of information no longer hold. Thus, with $\mathbf{v} = (\dot{q}, \dot{p})$, the integrand become

$$(p, q) \cdot (\dot{q}, \dot{p}) = p\dot{q} + q\dot{p} \tag{78}$$

Using that $q = \int dq$ and the Hamilton equation $\dot{p} = -\frac{\partial \mathcal{H}}{\partial q}$, the integrand can be written as

$$p\dot{q} - \int dq \frac{\partial \mathcal{H}}{\partial q} = p\dot{q} - \int d\mathcal{H} = p\dot{q} - \mathcal{H} \tag{79}$$

Equivalently, the integrand could have been written as

$$q\dot{p} + \mathcal{H} \tag{80}$$

by using that $p = \int dp$ and the other Hamilton equation $\dot{q} = \frac{\partial \mathcal{H}}{\partial p}$. However, the form $p\dot{q} - \mathcal{H}$ is the preferred choice due to the fact that it is equal to the Lagrangian $\mathcal{L}$. Thus,

$$\delta \int_{t_i}^{t_f} dt \int dS \; \mathcal{L} = 0 \tag{81}$$

The equality must hold independently on the surface area of the tube, i.e. the principle of information conservation should hold true independently on the number of states in which the system can exist. Therefore, the integration over the surface area can be taken outside of the infinitesimal variation, giving that

$$\delta \int_{t_i}^{t_f} dt \; \mathcal{L} = 0 \tag{82}$$

which is, again, Hamilton's principle.

Acknowledgement

The author would like to express gratitude to Anke Olsen for many inspiring discussions in our office at Bacchus.

References

1. Goldstein, H., Poole, C., Safko, J.: Classical mechanics. Addison-Wesley, 3rd ed. (2000)
2. Landau, L.D., Lifshitz, E.M.: Mechanics (Course of Theoretical Physics, vol.1.) Reed Educational and Professional Publishing, 3rd ed. (1976)
3. Hand, L.N., Finch, J.D.: Analytical Mechanics Cambridge University Press, 1st ed. (1998)
4. Greiner, W.: Classical Mechanics: Systems of Particles and Hamiltonian Dynamics Springer, 1st ed. (2003)
5. Lagrange, J.L.: Mecanique Analytique, vol. I. M.V. Courcier, 1st ed., Paris (1811)
6. Lagrange, J.L.: Mecanique Analytique, vol. II . Mallet-Bachelier, 3rd ed. , Paris (1815)
7. Hamilton, W.R.: On the application to dynamics of a general mathematical method previously applied to optics. British Association Report, pp. 513-518. Edinburgh (1834)
8. J.E. Moyal "Quantum mechanics as a statistical theory," Proceedings of the Cambridge Philosophical Society, **45**, p.99-124 (1949).
9. Gibbs, J.W.: Elementary principles in statistical mechanics. Charles Scribner's sons, New York (1902)
10. Bloch, F.: Fundamentals of statistical mechanics: manuscript and notes of Felix Bloch. Imperial College Press and World Scientific Publishing, 3rd ed., London (2000)
11. Jeffreys, H., Jeffreys B.S.: Methods of mathematical physics. Cambridge University Press, 3rd ed. (1956)