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On the Gibbs-Liouville theorem in classical mechanics

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

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Contents

1 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. In figure 1 examples of de-

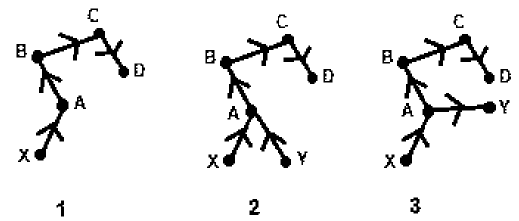

Fig. 1 Deterministic and non-deterministic evolution of a physical system.

terministic and non-deterministic evolution are shown. Evolution 1 represent deterministic motion both into the future and into the past. Consider e.g. state B. It is known with certainty that the previous state was A and that the next state will be C. Evolution 2 and 3, on the other hand, represent non-deterministic motions. Along evolution 2, it is known with certainty that state A will evolve into state B but it is uncertain whether it evolved from state X or Y. Hence, it is deterministic into the future but non-deterministic into the past. Evolution 3 is deterministic into the past but non-deterministic into the future. The reason for this is that it is impossible to say which of the states Y and B the state A will evolve into. The assumption of deterministic evolution thus imply that nowhere on phase space can states converge or diverge, see figure 2.

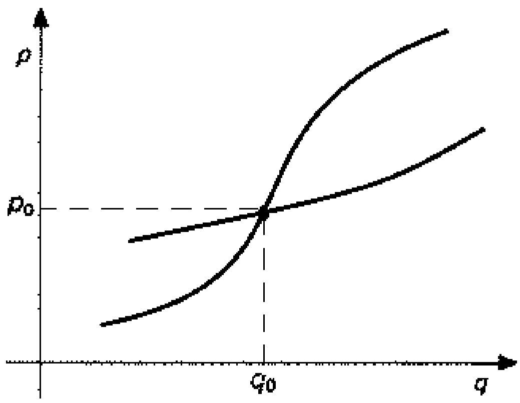

Fig. 2 A violation of the assumption of deterministic evolution imply that system trajectories would cross each other on phase space, here at point (q_0, p_0). In other words, nowhere on phase space can states converge or diverge.

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, e.g. state X in evolution 2, and evolve as $X \to A \to B \to C \to D$, it is not necessarily the case that the system end up at the same initial state X by reversing the motion of the system in time. It might be that, upon time-reversal, the system evolve as $D \to C \to B \to A \to Y$. 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.

In general, there are three sources for apparent violations of reversibility. It might be that microscopic degrees of freedom has been ignored, as is the case for the sliding block. Or it might be that the system is simply too big that it is not feasible to keep track of all the degrees of freedom. Or it might be that the system interact in complicated ways with an environment, whose degrees of freedom are difficult to take into account. In any case, if all the properties of a system is known to infinite precision, at any given time, the evolution of the system is reversible. On phase space, the time-reversed evolution of the system would follow the same trajectory as when evolving forward in time, with the difference that $p \to -p$.

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 about the system. This is 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. Thus, the loss of distinction between states imply that information has been lost. In conclusion, 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.

Thus, in conclusion, the assumption that classical systems evolve deterministically, i.e. that the state of the system is perfectly predictable 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. In the next section, it is argued that the Gibbs-Liouville theorem is a mathematical representation of the statement of information conservation.

2 The Gibbs-Liouville theorem

Consider an arbitrary region Ω on phase space, with volume V_Ω and infinitesimal volume element $dqdp$. That information is conserved within Ω put two requirements on the flow of states. First, the total number of states, N, within Ω is constant in time,

$$\frac{dN}{dt} = 0 \tag{1}$$

In other words, there can be no net increase or decrease in the number of states within Ω. Secondly, the set of N states is unique and stay the same for all times. The second requirement is needed to avoid the possibility that states are created and destroyed at the same rate at different locations on phase space. This is fulfilled if the density of states on phase space, $\rho(q,p,t)$, is constant in time,

$$\frac{d\rho}{dt} = 0 \tag{2}$$

When these two conditions are met, states on phase space cannot converge or diverge. Such a flow of states is referred to as an incompressible flow.

The number of states N is related to the density of states $\rho(q,p,t)$ by

$$N = \int_{V_\Omega} \rho(q,p,t)dqdp \tag{3}$$

The first condition thus become

$$\begin{aligned}\frac{dN}{dt} &= \frac{d}{dt}\int_{V_\Omega} \rho(q,p,t)dqdp \\ &= \int_{V_\Omega} \left(\frac{d\rho}{dt} + \rho\ \boldsymbol{\nabla}\cdot\mathbf{v}\right) dqdp \\ &= 0\end{aligned} \tag{4}$$

where

$$\boldsymbol{\nabla} = \left(\frac{\partial}{\partial q}, \frac{\partial}{\partial p}\right) \tag{5}$$

is the differential operator on phase space, and

$$\mathbf{v} = (\dot{q}, \dot{p}) \tag{6}$$

is the velocity by which states flow on phase space. Since information should be conserved independently on the size of Ω, the integrand in equation 4 must vanish for arbitrary volumes V_Ω, i.e.

$$\frac{d\rho}{dt} + \rho\ \boldsymbol{\nabla}\cdot\mathbf{v} = 0 \tag{7}$$

This is the continuity equation for the flow of states on phase space. It say that the number of states is locally conserved. This can be seen more explicitly by rewriting it as follows. The total time derivative of the density of states is

$$\frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial q}\dot{q} + \frac{\partial \rho}{\partial p}\dot{p} \tag{8}$$

$$= \frac{\partial \rho}{\partial t} + (\boldsymbol{\nabla}\rho) \cdot \mathbf{v} \tag{9}$$

Using the product rule

$$\boldsymbol{\nabla} \cdot (\rho \mathbf{v}) = (\boldsymbol{\nabla}\rho) \cdot \mathbf{v} + \rho \boldsymbol{\nabla} \cdot \mathbf{v} \tag{10}$$

the continuity equation is rewritten as

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \mathbf{v}) = 0 \tag{11}$$

The term $\boldsymbol{\nabla} \cdot (\rho \mathbf{v})$ represent the net flow of states through Ω, i.e. the difference between the outflow and inflow of states. The continuity equation state that if there is a net outflow of states, i.e. if

$$\boldsymbol{\nabla} \cdot (\rho \mathbf{v}) > 0 \tag{12}$$

then the density of states within Ω decrease with time, i.e.

$$\frac{\partial \rho}{\partial t} = -\boldsymbol{\nabla} \cdot (\rho \mathbf{v}) < 0 \tag{13}$$

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

$$\boldsymbol{\nabla} \cdot (\rho \mathbf{v}) < 0 \tag{14}$$

then the density of states within Ω increase with time, i.e.

$$\frac{\partial \rho}{\partial t} = -\boldsymbol{\nabla} \cdot (\rho \mathbf{v}) > 0 \tag{15}$$

In order for the flow of states on phase space to satisfy the principle of conservation of information, the density of states must be constant in time. From the continuity equation it is thus obtained that the divergence of the flow velocity must vanish, i.e.

$$\boldsymbol{\nabla} \cdot \mathbf{v} = 0 \tag{16}$$

In conclusion, if the divergence of the flow velocity vanish, the flow of states on phase space is incompressible and hence information is conserved. This is the mathematical representation, in differential form, of the principle of information conservation. It can be restated in terms of volumes on phase space. Consider a group, any group, of N states on phase space. Due to the incompressibility of the flow of states on phase space, with each state having a volume dV, the total volume $V = \sum_{j=1}^{N} dV_j = N \cdot dV$ of the group of N states remain constant in time as they flow on phase space. This conclusion is the Gibbs-Liouville theorem [1][2]. The continuity equation is the Gibbs-Liouville equation for the density of states on phase space.

3 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

$$\frac{\partial \dot{q}}{\partial q} + \frac{\partial \dot{p}}{\partial p} = 0 \tag{17}$$

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 [8],

$$\dot{q} = \frac{\partial \mathcal{H}}{\partial p} \tag{18}$$

$$\dot{p} = -\frac{\partial \mathcal{H}}{\partial q} \tag{19}$$

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.

4 The Hamiltonian and Lagrangian

The Hamilton equation 18 correspond to the integral equation

$$\mathcal{H}(p) = \int dp\ \dot{q}(p) \tag{20}$$

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 3. Due to the one-to-one correspondence between p and $\dot{q}$ it is possible to define a

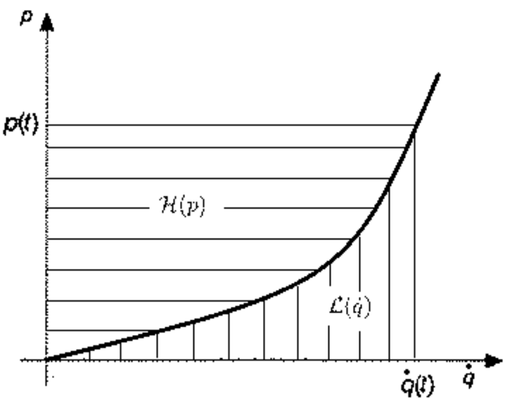

Fig. 3 The areas under $\dot{q}(p)$ and $\dot{p}(q)$ graphs define the Hamiltonian and Lagrangian, respectively.

related area, $\mathcal{L}(\dot{q})$, given by the unique area under the $p(\dot{q})-$graph,

$$\mathcal{L}(\dot{q}) = \int d\dot{q}\ p(\dot{q}) \tag{21}$$

This integral equation correspond to the differential equation[1]

$$\frac{d\mathcal{L}(\dot{q})}{d\dot{q}} = p \tag{22}$$

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

$$\mathcal{L}(\dot{q}) + \mathcal{H}(p) = p \cdot \dot{q} \tag{23}$$

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,

$$\mathcal{L}(q, \dot{q}) + \mathcal{H}(q, p) = p \cdot \dot{q} \tag{24}$$

where

$$\mathcal{L}(q, \dot{q}) = \int_0^{\dot{q}} d\dot{q}\ p(\dot{q}) - U(q) \tag{25}$$

$$\mathcal{H}(q, p) = \int_0^{p} dp\ \dot{q}(p) + U(q) \tag{26}$$

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.

5 Principle of stationary action

The Hamilton equations

$$-\frac{\partial \mathcal{H}}{\partial q} - \dot{p} = 0 \tag{27}$$

$$\dot{q} - \frac{\partial \mathcal{H}}{\partial p} = 0 \tag{28}$$

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 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,

$$\left(-\frac{\partial \mathcal{H}}{\partial q} - \dot{p}\right)\delta q(t) = 0 \tag{29}$$

$$\left(\dot{q} - \frac{\partial \mathcal{H}}{\partial p}\right)\delta p(t) = 0 \tag{30}$$

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

$$q(t) \to q(t) + \delta q(t) \tag{31}$$

$$p(t) \to p(t) + \delta p(t) \tag{32}$$

Equations 29 and 30 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

$$\delta q(t_i) = \delta q(t_f) = 0 \tag{33}$$

$$\delta p(t_i) = \delta p(t_f) = 0 \tag{34}$$

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,

$$\int_{t_i}^{t_f} dt\ \left[\left(-\frac{\partial \mathcal{H}}{\partial q} - \dot{p}\right)\delta q(t) + \left(\dot{q} - \frac{\partial \mathcal{H}}{\partial p}\right)\delta p(t)\right] = 0 \tag{35}$$

Integration by parts and recalling the boundary conditions give

$$\begin{aligned} 0 &= \int_{t_i}^{t_f} dt\ \left[\frac{\partial(\dot{q}p - \mathcal{H})}{\partial q} - \frac{d}{dt}\frac{\partial(\dot{q}p - \mathcal{H})}{\partial \dot{q}}\right]\delta q(t) \\ &+ \int_{t_i}^{t_f} dt\ \left[\frac{\partial(\dot{q}p - \mathcal{H})}{\partial p} - \frac{d}{dt}\frac{\partial(\dot{q}p - \mathcal{H})}{\partial \dot{p}}\right]\delta p(t) \\ &= \int_{t_i}^{t_f} dt\ \delta\left(\dot{q}p - \mathcal{H}\right) \\ &= \delta\int_{t_i}^{t_f} dt\ \left(\dot{q}p - \mathcal{H}\right) \\ &= \delta\int_{t_i}^{t_f} dt\ \mathcal{L} \\ &= \delta\mathcal{A} \end{aligned} \tag{36}$$

where

$$\mathcal{A} \equiv \int_{t_i}^{t_f} dt\ \mathcal{L} \tag{37}$$

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

[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 [9].

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

$$\delta \mathbf{v} = \mathbf{v}(q + \delta q, p + \delta p) - \mathbf{v}(q, p) = \delta q \frac{\partial}{\partial q}\mathbf{v} + \delta p \frac{\partial}{\partial p}\mathbf{v} \tag{38}$$

The divergence of the flow velocity transform as

$$\boldsymbol{\nabla} \cdot \mathbf{v} \to \boldsymbol{\nabla} \cdot (\mathbf{v} + \delta \mathbf{v}) = \boldsymbol{\nabla} \cdot \mathbf{v} + \boldsymbol{\nabla} \cdot \delta \mathbf{v} \tag{39}$$

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

$$\boldsymbol{\nabla} \cdot \delta \mathbf{v} = 0 \tag{40}$$

which is equivalent to

$$\delta \left(\boldsymbol{\nabla} \cdot \mathbf{v} \right) = 0 \tag{41}$$

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,

$$\delta \int_{t_i}^{t_f} dt \int_V dV \ \boldsymbol{\nabla} \cdot \mathbf{v} = 0 \tag{42}$$

Applying the divergence theorem

$$\int_V dV \ \boldsymbol{\nabla} \cdot \mathbf{v} = \int_{\partial V} \mathbf{dS} \cdot \mathbf{v} \tag{43}$$

give

$$\delta \int_{t_i}^{t_f} dt \int_{\partial V} \mathbf{dS} \cdot \mathbf{v} = 0 \tag{44}$$

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

$$\mathbf{dS} = dS \ \mathbf{n} \tag{45}$$

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

$$(p, q) \cdot (\dot{q}, \dot{p}) = p\dot{q} + q\dot{p} \tag{46}$$

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

$$p\dot{q} - \int dq \frac{\partial \mathcal{H}}{\partial q} = p\dot{q} - \int d\mathcal{H} = p\dot{q} - \mathcal{H} \tag{47}$$

Equivalently, the integrand could have been written as

$$q\dot{p} + \mathcal{H} \tag{48}$$

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,

$$\delta \int_{t_i}^{t_f} dt \int dS \ \mathcal{L} = 0 \tag{49}$$

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

$$\delta \int_{t_i}^{t_f} dt \ \mathcal{L} = 0 \tag{50}$$

which is, again, Hamilton's principle.

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