Liouville’s Theorem

PHGN 505 Report

by

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1 Introduction and Basic Formulation

Liouville’s theorem describes the evolution of the distribution function in phase space for a Hamiltonian system. It is a fundamental theory in classical mechanics and has a straightforward generalization to quantum systems. The basic idea of Liouville’s theorem can be presented in a basic, geometric fashion. The mathematical derivation is also rather straightforward. Liouville’s theorem applies to all Hamiltonian systems with number of particles. The single particle case is important but rather boring. The theorem becomes more important in classical statistical mechanics as the particle number becomes very large. In particular, Liouville’s theorem, along with its partners ergodicity, entropy, and Poincare’s recurrence theorem, describe the equilibration and fluctuations of a dynamical system. This report is based in classical mechanics, but because of the utility of Liouville’s theorem in many particle physics, it includes many ideas from statistical mechanics. References [3] [5] [4] [2] [1] are listed in arbitrary order.

$N$ particles in a Hamiltonian system can be described by their position in phase space, the $6N$ dimensional space with 3 coordinate axes and 3 momentum axes. A particle’s location in phase space is equivalent to specifying its position and momentum. Trajectories through phase space, then, are the dynamical paths taken by particles in the system. Because phase space is cartesian, its volume element can be written $dV_\text{phase} = dx\,dy\,dz\,dp_x\,dp_y\,dp_z$ with units $m^3 (N s)^3$. The distribution function $f(r, p, t)$ relates phase space volume elements to the number of particles in that volume. In differential form, this takes the form

$$dN = f(r, p, t) \, dx\,dy\,dz\,dp_x\,dp_y\,dp_z = f(r, p, t) \, d^3x \, d^3p \quad (1)$$

Again, the distribution function $f$ is the number of volume elements occupying the differential phase space volume $d^3x \, d^3p$.

Liouville’s theorem is concerned with the time evolution of distribution functions. We start this discussion by considering the simplest case of a collection free particles. If the initial conditions of the problem dictate that the occupied volume in phase space is a hypercube, how does the system evolve? States farthest from the origin in the direction of momentum will shift the most as the system evolves. This is not due to any external forces, only the initial conditions causing the hypercube to distort. States closer to the origin will shift less, and the cube will be a distorted 6 dimensional parallelogram with its center shifted along the position axes from its initial position. As certain corners of the distribution shift further from each other, opposite pairs of corners shift closer together. The distribution is effectively stretched in the direction with the greatest initial momentum. The volume, particle number, and phase space density all remain constant as in the zero force case.
The constant density of particles in phase space is one loosely worded version of Liouville’s theorem.

## 2 Derivation of Boltzmann Equation and Liouville’s Theorem

Continuity equations describe the rate of change of particles at a point in space as a function of the particle velocities, density gradients, forces, and any particle sources or sinks. First consider the steady flow of a fluid through space. The total number of particles in a closed surface is found by integrating the particle density over the volume of the surface. For the number of particles in the volume to change in time, there must be a net flux of particles in or out of the surface. Integrating the velocity at any time over the surface of the sphere gives the following relation

\[
\frac{\partial N}{\partial t} = - \int \int n \mathbf{v} \cdot d\mathbf{S} \tag{2}
\]

where \( n \) is the particle density. After applying Gauss’ theorem, one obtains the well known continuity equation.

\[
\frac{\partial n}{\partial t} = - \nabla \cdot (n \mathbf{v}_b) \tag{3}
\]

The rate of change of the density depends on the sources of particles. This can be straightforwardly generalized to 6\(N\) dimensional phase space by replacing \( \nabla \) with a 6 dimensional divergence - 3 coordinate and 3 momentum derivatives. Expanding the derivatives gives Eq. 4.

\[
\frac{\partial f}{\partial t} = - \mathbf{v} \cdot \nabla f - f \nabla \cdot \mathbf{v} - \mathbf{F} \cdot \nabla p f - f \nabla p \cdot \mathbf{F} \tag{4}
\]

The \( \nabla \cdot \mathbf{v} \) term can be discarded. This divergence is three partial derivatives over position, keeping all other variable constant. Since the \( p_i \) are held constant, the \( v_i \) are as well and this term is zero. We discard another term in this equation with the common restriction of conservative systems. If the \( p \)-divergence of the force is zero, we can discard the fourth term on the right side. In other words, the force cannot depend on momentum, i.e. conservative.
forces only from this point on in the derivation. Adding a collision term of the form $\delta f/\delta t$ gives the Boltzmann transport equation, which is useful in its own right. Excluding the collision term will lead to Liouville’s theorem, however. Generalizing the remaining terms to multiple particles, and recognizing the velocity as $dx/dt$ and force as $dp/dt$, one gets the Liouville equation.

$$\frac{\partial f}{\partial t} + \sum_i \frac{\partial f}{\partial x_i} \frac{dx_i}{dt} + \sum_i \frac{\partial f}{\partial p_i} \frac{dp_i}{dt} = 0$$

Eq. 5 can be recognized as the total derivative of the distribution function $f$. Indeed, Liouville’s theorem says the density of a vanishingly small element of phase space is conserved in time as it is followed around a phase space trajectory. The partial derivative equates explicit time changes in the distribution function to the forces on the system and the instantaneous velocities - this is true if one observes a fixed surface in phase space and allows density to flow through it. The total derivative, on the other hand, tracks the time evolution of the coordinates as well, not only the distribution function. Thus, Liouville’s theorem states that the phase space density of a certain element as it moves in phase space is fixed, $df/dt = 0$.

One can return to the geometric argument presented in the first section as well. Conservation of particles in phase space requires

$$\frac{d}{dt}(f(r,p,t)d^3x d^3p) = 0$$

Applying the chain rule to the derivative above, we see that $\frac{d}{dt}d^3xd^3p = 0$ since $f$ can take arbitrary values. This alternative statement of Liouville’s theorem is that the volume occupied by a given set of particles is conserved as one tracks the particles through phase space. This is exactly the conclusion drawn from the simple hypercube evolution in the previous section. These two definitions can be combined as the condition of incompressible flow in phase space. Analogously and perhaps more intuitively in fluid mechanics, incompressible flow occurs under the condition $d\rho/dt = 0$ for density $\rho$. This behavior can be seen in either statement of Liouville’s theorem - small volumes in phase space can be twisted and stretched, but can never be destroyed.

3 Alternative Derivation

Phase space is the $6N$ dimensional space describing the position and momentum of each of the $N$ particles of a dynamical system. At any time $t$, the system is wholly described by its configuration in phase space, denoted $P(\vec{q}, \vec{p})$ for $3N$ dimensional vectors $\vec{q}$ and $\vec{p}$. At a later time $t'$, the system will evolve to a new configuration $P(\vec{q}', \vec{p}')$ given by integrating Hamilton’s equations. In this manner, the new phase space coordinates $\vec{q}'$ and $\vec{p}'$ can be considered a function of the previous coordinates at $t$. The phase space volume elements at different times can be related by Eq. 7.

$$dV' = J(t,t')dV$$

$J(t,t')$ is the Jacobian determinant of the transformation, i.e.

$$J(t,t') = \frac{\partial(\vec{q}_k', \vec{p}_k')}{\partial(\vec{q}_i, \vec{p}_i)}$$
$J(t, t')$ uses the transformations of individual coordinates to describe the transformation of the entire volume element $dV$. If $t = t'$, then $\vec{p}_k = \vec{p}'_k$ and $\vec{q}_k = \vec{q}'_k$, meaning only the diagonal elements of the Jacobian matrix survive. This leaves the identity $J(t, t) = 1$, a pleasing result.

Now let $t' = t + dt$ and keep terms first order in $dt$. Hamilton’s equations give the following.

\begin{align*}
\dot{p}_k &= \frac{dp_k}{dt} = -\frac{\partial H}{\partial q_k} \quad (9) \\
\dot{q}_k &= \frac{dq_k}{dt} = -\frac{\partial H}{\partial p_k} \quad (10) \\
p'_k &= p_k - \frac{\partial H}{\partial q_k} dt \quad (11) \\
q'_k &= q_k + \frac{\partial H}{\partial p_k} dt \quad (12)
\end{align*}

Evaluating the determinant in Eq. 7 to first order in $dt$ to get $J(t, t + dt)$ gives Eq. 14.

\[ J(t, t + dt) \approx 1 + \sum_k \left( \frac{\partial^2 H}{\partial p_k q_k} - \frac{\partial^2 H}{\partial p_k q_k} \right) dt = 1 \quad (13) \]

\[ J(t, t + dt) = J(t, t) + \frac{\partial}{\partial t} J(t'', t) \bigg|_{t''=t} dt = 1 \quad (14) \]

The second line in Eq. 4 is a simple taylor expansion for infinitesimal distance $dt$ away from time $t$. We previously showed that $J(t, t) = 1$. Together, these results tell us that

\[ \frac{\partial}{\partial t'} J(t'', t) \bigg|_{t''=t} = 0 \quad (15) \]

This is a key element in this derivation of Liouville’s theorem. Remembering that $J(t, t')$ describes the transformation of some phase space volume from $dV'$ to $dV''$, we can write a composite transformation as a product of $J$’s.

\[ dV' = J(t, t'') J(t'', t') dV = J(t, t') dV \quad (16) \]

The composite transformation can be written $J(t, t') = J(t, t'') J(t'', t')$. Now take the derivative of $J(t, t')$ with respect to $t'$ and evaluate at $t'' = t'$.

\[ \frac{\partial J(t, t')}{\partial t'} = J(t, t'') \frac{\partial}{\partial t'} J(t'', t') \bigg|_{t''=t'} \quad (17) \]

Eq. 15 implies that the partial derivative on the right side of Eq. 17 is zero, since Eq. 15 holds for arbitrary time $t$. Since the right side of Eq. 17 equals zero, so must the left side.

\[ \frac{\partial}{\partial t'} J(t, t') = 0 \quad (18) \]
Eq. 18 describes the time evolution of $J$ for arbitrary values of $t$ and $t'$. This is a first order differential equation for the jacobian determinant. The initial condition at $t' = t$ is $J(t, t) = 1$. Since the transformation $J(t, t')$ does not change with respect to the final time $t'$ by Eq. 18, $J(t, t') = 1$ for all times $t'$. Since $J(t, t')$ is the transformation of differential volumes in phase space, we conclude that $dV' = dV$. The magnitude of an arbitrary, differential volume element in phase space does not change along its trajectory through phase space. This is Liouville’s theorem.

The same result holds for any finite, closed volume in phase space along the phase space trajectories. For every infinitesimal volume element $dV$ in some finite region $R$ there is a corresponding equal volume element $dV'$ at a later time $t'$ dictated by the equations of motion. This is a more fundamental derivation of Liouville’s theorem than discussed previously. A simple example helps illustrate the utility of this transformation method. Consider a free particle in one dimension. Hamilton’s equations give time evolution according to

$$\dot{p} = -\frac{\partial H}{\partial q} = 0 \quad \text{(19)}$$
$$\dot{q} = \frac{\partial H}{\partial p} = \frac{p}{m} \quad \text{(20)}$$

Integrating these equations gives $p = \text{constant}$ and $q = (p/m)t$. In the previous notation of transformations from $t$ to $t'$, the evolution is

$$p' = p \quad \text{(21)}$$
$$q' = q + \frac{p}{m}(t' - t) \quad \text{(22)}$$

The Jacobian of this transformation is readily evaluated in Eq. 23.

$$J(t, t') = \begin{vmatrix} \frac{\partial p'}{\partial p} & \frac{\partial p'}{\partial q} \\ \frac{\partial q'}{\partial p} & \frac{\partial q'}{\partial q} \end{vmatrix} = \begin{vmatrix} 1 & \frac{t' - t}{m} \\ 0 & 1 \end{vmatrix} = 1 \quad \text{(23)}$$

This is a specific example of the general result to illustrate the application of Liouville’s theorem. Constructing the determinant $J(t, t')$ quickly becomes an impossible task for larger systems with multiple particles.

4 Example: Photons in Phase Space

To illustrate the versatility of Liouville’s theorem, we consider the application to massless particles. Liouville’s theorem correctly describes a number of properties associated with light propagation, including brightness and specific intensity.

We start with the usual prescription of describing the distribution of a system of $N$ photons in phase space. The distribution in phase space is given by

$$dN = f(r, p, t)d^3r d^3p \quad \text{(24)}$$
It is helpful for radiative systems to switch to spherical coordinates. In this coordinate system, the differential elements are as follows.

\[
d^3p = p^2 dp d\Omega = \frac{1}{c^3} E^2 dE d\Omega \quad (25)
\]

\[
d^3r = cdxdydt = cd^2 \Sigma dt \quad (26)
\]

\(d\Omega\) is the solid angle subtended by the photons. The substitution in the first line of Eq. 26 uses the fact that \(p\) is proportional to \(E\) for photons, i.e. massless particles have linear dispersion. Because the particles all travel with speed \(c\), the differential volume occupied by the particles is related to the flux over a differential area \(d^2 \Sigma\) multiplied by a differential time \(dt\). By simple dimensional analysis, one can confirm that the second equation in Eq. 26 has the proper units of volume. By conservation of phase space volume (Liouville's theorem), we can see that the product of spatial density with momentum density must be constant. Close to a light source, a ray of photons occupies a small physical volume (high density), but their relative trajectories are distributed across several momentum vectors (low momentum density). Far from a light source, a ray of photons is diffuse in physical space (low density), but highly collimated in direction (high momentum density). Therefore, dilution of photon density is always paired with increased collimation - their product must be constant. This characteristic is reminiscent of something like a classical uncertainty principle for a collection of particles. If you squeeze particles together in space, their spread in momentum space increases.

Let’s use these phase space relationships to compute the total photon energy density in a small volume of phase space. Let \(d\epsilon\) denote the differential energy in a small volume of phase space.

\[
d\epsilon = f(\mathbf{r}, \mathbf{p}, t) E d^3 x d^3 p = Ef(\mathbf{r}, \mathbf{p}, t)(cd^2 \Sigma dt)(\frac{1}{c^3} E^2 dE d\Omega) = Id^2 \Sigma dt dEd\Omega \quad (27)
\]

The specific intensity \(I\) is defined as \(I = f(\mathbf{r}, \mathbf{p}, t)E^2/c^2\). Because the distribution function \(f\) is conserved by Liouville’s theorem and \(E\) is constant for each photon, specific intensity \(I\) is also conserved. If you look at a light source while moving farther away from it, its “surface brightness” is constant. This is a well known effect we have all experienced - the radiated energy is constant over any area of interest. This is explained fundamentally by Liouville's theorem. This has some interesting consequences in optics. For instance, no telescope, however large, can make an object look brighter - it can only make it look larger. We have used the notion of photons here, but it is not essential to the physics and the explanation is equivalent for classical radiation. Fig. 2 shows the variation of the occupied phase space volume for three different distances away from a radiating source. The distortion at different distances (and equivalently, times) is similar to the initial example discussed in section 1. At the nearest distance (A), the photons are concentrated in a relatively small volume of position space. At the furthest distance (C), the spread in position is large, corresponding to a low density in position space. Small horizontal slices of each parallelogram correspond to particles at the same momentum. As the distance from the source increases from A to C,
Figure 2: Displacement in phase space of a collection of photons some distance away from their source.

the number of particles in a single horizontal slice increases. The photons become collimated at large distances. As the distance approaches infinity, the parallelogram approaches a thin horizontal rectangle along the position axis - the photons are perfectly collimated with a large spread in their position.

5 Ergodicity

As the number of particles in a Hamiltonian system becomes very large, statistical averages over microstates become meaningful. As a result, Liouville’s theorem has interesting implications in statistical mechanics. An ergodic system is one that is thoroughly mixed by time evolution. All components of phase space pass arbitrarily close to other points of the constant energy surface in an ergodic system. This is the reason that time averages of statistical quantities are assumed equal to averages of the corresponding microcanonical ensemble. An ergodic system is very well “stirred” by time; over long enough time scales, all microstates of constant energy are accessed. An alternative definition of ergodicity examines a vanishingly small fraction of the energy surface. Define an element \( R \) of the energy surface \( S \) that remains invariant under phase space flow. The set \( R \) is independent of time evolution.

A system is ergodic if and only if the element \( R \) has zero volume or has a volume equal to that enclosed by the surface \( S \). If any finite volume of phase space is not mixed with the rest of the energy surface, the system is not ergodic.

The connection between ensemble averages and temporal averages is important to our interpretation of experimental results. Physicists cannot typically measure an ensemble of identical systems at the same time started from the same initial conditions to determine the equilibrium state. This would be a true ensemble average. Instead, we measure the same system several times to draw conclusions about its equilibrium state. Because an ergodic system is guaranteed to explore all microstates of the system, a continuous temporal measurement
over something akin to the “period” of the system is equivalent to the true ensemble average. This idea is closely related to Poincare’s recurrence theorem, to be discussed later. These measurements include even extreme fluctuations away from what is considered equilibrium. Again, the ergodic hypothesis is that temporal averages are equivalent to microcanonical ensemble averages, a consequence of Liouville’s theorem. Eq. 31 represents this relationship mathematically.

\[
\langle f \rangle = \int_{\Gamma} f(x) d\mu(x) \quad \text{(30)}
\]

\[
= \bar{f} = \frac{1}{T} \int_{0}^{T} dt f(x(t)) \quad T \to \infty \quad \text{(31)}
\]

\[d\mu(x)\] is the integration measure for phase space. While ergodicity is a fairly intuitive concept, it is usually difficult to prove for a real system. Often, it is taken as a postulate of a system so experimental results are meaningful in the previous temporal/ensemble average context. In practice, this has been proven for relatively few systems (among them collisions of hard spheres and geodesic motion on finite surfaces with constant negative curvature). A system with multiple disjointed surfaces in phase space, all at a constant energy, is not ergodic since it is discontinuous. The topology of the energy surface can reveal much about the ergodicity or validity of Liouville’s theorem, as well as the validity of Poincare’s recurrence theorem (to be discussed later). I cannot think of any physical systems this specific example represents, but there certainly are non-ergodic systems. Ferromagnets and glassy systems are two examples of such non-ergodic systems. In both cases, the system is able to explore only a subset of all equal energy states, though it explores this subset ergodically.

## 6 Poincare Recurrence Theorem

Because Liouville’s theorem is so fundamental and versatile in classical statistical mechanics, it is not surprising it is an important component of other theories related to entropy, reversibility, and ergodicity (previously discussed). One example of a conjecture that hinges on Liouville’s theorem is Poincare’s recurrence theorem. Poincare’s theorem states that, for a large class of systems, a dynamical system will return arbitrarily close to its initial state after sufficiently long time.

Let the state of a dynamical system be represented by the point \( \mathbf{r} \) in phase space. Let \( g_0 \) be an arbitrary volume element contained in the phase space volume \( V_0 \). After some time \( t \), all points in \( g_0 \) will evolve into another volume element \( g_t \) in a volume \( V_t \), determined by the initial conditions and equations of motion. For a Hamiltonian system, Liouville’s theorem applies and \( V_0 = V_t \). Let \( \Gamma_0 \) denote the subspace of phase space that is the union of all \( g_t \) for all \( 0 < t < \infty \). Let the volume of \( \Gamma_0 \) be \( \Omega_0 \). Analogously, \( \Gamma_0 \) is the subspace that is the union of all \( g_t \) for all \( \tau < t < \infty \). Let its volume be \( \Omega_\tau \). Since the energy is finite, and assuming the spatial volume of the system is finite, both \( \Omega_0 \) and \( \Omega_\tau \) are finite. These definitions imply that \( \Gamma_0 \) contains \( \Gamma_\tau \), since it is permissible for \( \tau \) to run from \( 0 < \tau < \infty \). If \( \Gamma_0 \) is occupied by the distribution function of the system \( f(\mathbf{r}, \mathbf{p}, t) \) and allowed to evolve, it is obvious that after time \( \tau \), \( \Gamma_0 \) will become \( \Gamma_\tau \). Liouville’s theorem mandates that the volume of the phase space element is invariant, \( \Omega_0 = \Omega_\tau \).
Recall that $\Gamma_0$ contains $\Gamma_\tau$. That is, all states evolved from $g_0$ are contained in $\Gamma_0$. Because $\Omega_0$ has the same volume as $\Omega_\tau$, we conclude that $\Gamma_0$ and $\Gamma_\tau$ contain the same set of points. Because $\Gamma_\tau$ contains all initial configurations $g_0$, at least one future state $g_\tau$ is equal to the initial state $g_0$. Therefore, all points in the element $g_0$ must return to $g_0$ after some sufficiently long time.

This is a powerful theorem related to entropy and fluctuations about equilibrium. It is similar in flavor to microcanonical ensembles where all microstates are accessible with some nonzero probability. Poincare’s recurrence theorem says that the initial state, no matter how far from equilibrium, will still be accessed after some time. This is observed as a fluctuation from equilibrium, and is clearly in agreement with the assumptions of microcanonical statistical mechanics. An alternate formulation of the proof relies on two assumptions: volume of a finite phase space element is conserved (Liouville’s theorem) and phase space trajectories do not intersect. We have already discussed in detail the first assumption. The second assumption is a reasonable physical assumption, analogous to non-crossings of field lines. If the trajectories did intersect, a phase space configuration placed at the intersection would have multiple trajectories. This is not allowed in deterministic classical mechanics. With these two assumptions in mind, imagine a small volume of phase space sweeping out its trajectory. Because the total volume is finite, and trajectories are not allowed to cross, after some time the volume must return to its initial location. In other words, the system will always return to its initial state. Poincare’s theorem does not necessarily require ergodicity. The volume element sweeping out its trajectory need not pass arbitrarily close to all other elements. In other words, the system can return to its initial conditions before exploring all of phase space. A simple picture of this is two disconnected phase space volumes. An initial condition in one volume needs only to explore all elements in its home volume before returning to its initial state.

For an ideal gas, assume that $N$ particles are initially in one corner of a box. Eventually, the system must return to this Delta-function behavior if Poincare’s theorem is true. The number of microstates available to the gas scales like $V^N$ for box volume $V$. If the volume of the initial corner is $v$, the probability of observing the system return to the initial state is roughly $(v/V)^N$. For $N$ on the order of $10^{23}$ and the initial volume as half the total volume, $v = V/2$, the Poincare recurrence time is $(V/v)^N \approx 2^{10^{23}}$ seconds. If one could observe the box for this length of time, one would see all the gas particles spontaneously arrange themselves into half of the box volume. This is certainly a rare fluctuation, commonly handled with other methods of classical statistical mechanics.

7 Second Law of Thermodynamics

Liouville’s theorem can be used to construct a proof of the second law of thermodynamics, originally attributed to Jaynes. Each microstate of a Hamiltonian system is specified in $6N$ dimensional phase space by the coordinate and momentum vectors $\mathbf{r}$ and $\mathbf{p}$. For every microstate specified by $\{\mathbf{r}, \mathbf{p}\}$ there exists a mirror microstate $\{\mathbf{r}, -\mathbf{p}\}$ with opposite momentum. Experimentally, we often have limited (or zero) knowledge of the microstate of the system - we see only the macrostate. Allow $W(A)$ to denote the phase volume of macrostate $A$, i.e. $W(A)$ is the number of microstates that realize macrostate $A$. We can
immediately conclude that $W(RA) = W(A)$. Consider two distinct macrostates $A$ and $B$ in the same phase space. Let $\Gamma$ denote the microscopic path through phase space that realizes the macroscopic transition $A \to B$. Denote the transformed macrostate $A$ as $TA$ for time evolved $A$. Liouville’s theorem preserves phase space volumes. Therefore, $W(TA) = W(A)$. We now consider only cases where the transition $A \to B$ is experimentally reproducible. For this to be true, $TA$ must lie entirely in $B$. We cannot control which microstate the system evolves into, but we require that all evolved microstates $TA$ are a subset of $B$. This condition implies that $W(TA) < W(B)$. The number of microstates for macrostate $B$ is greater than that of macrostate $A$. But Liouville’s theorem tells us $W(TA) = W(A)$, so experimental reproducibility of $A \to B$ means that $W(A) < W(B)$. This condition depends only on the initial configuration of the system because phase space volume is conserved. This is the requirement for experimental reproducibility and one explanation for entropy, $S \propto \ln W$. Consider the reverse transition: why does macrostate $B$ not evolve into $A$. This is equivalent to the transition $RB \to RA$. This transition requires additional information about the initial microstate of $RB$ to transform it into the proper sub-region of $RA$ - information we don’t typically have. Because $W(RA) < W(RB)$, this transformation is not experimentally reproducible. Liouville’s theorem connects the time evolved state to the initial state - their phase space volume are the same. Therefore, Liouville’s theorem places the requirement for experimental reproducibility (second law) on initial and final states $S(A) < S(B)$. Interestingly, nowhere does any notion of time enter this argument. In this derivation, increasing entropy is a requirement only for experimental reproducibility, not a forward direction in time.

Figure 3: Evolution of macrostates in a dynamical system.
8 Quantum Connection

Liouville’s theorem can be restated in terms of Poisson brackets, providing a useful connection to quantum mechanics. Equation 5 can be rewritten using Poisson bracket notation, where

\[
\{A, B\}_P = \sum_{\alpha} \frac{\partial A}{\partial q_\alpha} \frac{\partial B}{\partial p_\alpha} - \frac{\partial A}{\partial p_\alpha} \frac{\partial B}{\partial q_\alpha}
\]  
(32)

Recognizing that velocities can be reexpressed as \(\dot{q} = \partial H/\partial p\) and momenta as \(\dot{p} = -\partial H/\partial q\), Liouville’s theorem takes the form of Eq. 33.

\[
\frac{\partial f}{\partial t} = -\sum_{\alpha} \left( \frac{\partial f}{\partial q_\alpha} \frac{\partial H}{\partial p_\alpha} - \frac{\partial f}{\partial p_\alpha} \frac{\partial H}{\partial q_\alpha} \right) = -\{H, f\}_P
\]  
(33)

The time evolution of the distribution function is given by the Poisson bracket of the Hamiltonian with the distribution function. One correspondence between classical and quantum mechanics is the replacement of Poisson brackets in classical mechanics by commutators in quantum mechanics. Replacing the Poisson bracket in Eq. 33 with the commutator (and dividing by \(i\hbar\)) gives the quantum Liouville theorem. Quantizing the equation yields the Von Neumann equation, which describes the time evolution of quantum mixed state. In the quantum case, \(f\) must be replaced with the density matrix \(\rho\). Both \(H\) and \(\rho\) are now operators, as per the usual classical-quantum transition. When the quantum Liouville theorem is applied to the expectation value of an observable, the corresponding equation is known as Ehrenfest’s theorem, shown in Eq. 34.

\[
\frac{d}{dt} \langle A \rangle = \frac{1}{i\hbar} \langle [A, H] \rangle
\]  
(34)

Eq. 34 gives the time evolution of the expectation value of the operator \(A\). Expectation values of operators that commute with the Hamiltonian, then, do not change in time. This is the origin of stationary states in quantum mechanics. Thus, the quantum Liouville theorem, derived from the same principles as the classical counterpart, dictates the time evolution of operators, expectation values, and density operators in quantum mechanics.
References


